2-METHYLDOCOSANE

Other names: Docosane, 2-methyl
Inchi: InChI=1S/C23H48/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(2)3/h23H
InchiKey: AISQJRLSHDWVGU-UHFFFAOYSA-N
Formula: C23H48
SMILES: CCCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 324.64
CAS: 1560-81-2

Physical Properties

Property code	Value	Unit	Source
af	0.9352		Cheméo Relay (1.0)
gf	140.34	kJ/mol	Joback Method
hf	-535.79	kJ/mol	Cheméo Relay (1.0)
hfus	51.80	kJ/mol	Joback Method
hvap	113.34	kJ/mol	Cheméo Relay (1.0)
ie	9.98	eV	Cheméo Relay (1.0)
log10ws	-9.44		Cheméo Relay (1.0)
logp	9.074		Crippen Method
mcvol	334.930	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	2264.00		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2265.10		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2265.00		NIST Webbook
tb	597.27	K	Cheméo Relay (1.0)
tc	764.95	K	Cheméo Relay (1.0)
tf	304.68	K	Cheméo Relay (1.0)
vc	1.342	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1127.28	J/mol×K	864.55	Joback Method
cpg	1145.09	J/mol×K	892.42	Joback Method
cpg	1047.11	J/mol×K	753.07	Joback Method
cpg	1068.56	J/mol×K	780.94	Joback Method
cpg	1089.04	J/mol×K	808.81	Joback Method
cpg	1108.60	J/mol×K	836.68	Joback Method
cpg	1024.67	J/mol×K	725.20	Joback Method
dvisc	0.0004278	Pa×s	464.38	Joback Method
dvisc	0.0010359	Pa×s	399.17	Joback Method
dvisc	0.0035428	Pa×s	333.97	Joback Method
dvisc	0.0002197	Pa×s	529.59	Joback Method
dvisc	0.0001306	Pa×s	594.79	Joback Method
dvisc	0.0000860	Pa×s	659.99	Joback Method
dvisc	0.0000611	Pa×s	725.20	Joback Method
hvapt	79.70	kJ/mol	573.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45820e+01
Coeff. B	-4.95654e+03
Coeff. C	-1.50650e+02
Temperature range (K), min.	497.40
Temperature range (K), max.	685.30

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1560812&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume