Docosane, 3-methyl

Other names: 3-methyldocosane
Inchi: InChI=1S/C23H48/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(3)5-2/h23H
InchiKey: KYNAMBZEFDQTOF-UHFFFAOYSA-N
Formula: C23H48
SMILES: CCCCCCCCCCCCCCCCCCCC(C)CC
Mol. weight [g/mol]: 324.63

Physical Properties

Property code	Value	Unit	Source
gf	140.34	kJ/mol	Joback Method
hf	-523.33	kJ/mol	Joback Method
hfus	51.80	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	9.074		Crippen Method
mcvol	334.930	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2269.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2274.30		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2274.00		NIST Webbook
rinpol	2269.00		NIST Webbook
tb	725.20	K	Joback Method
tc	892.42	K	Joback Method
tf	333.97	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.67	J/mol×K	725.20	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	1127.28	J/mol×K	864.55	Joback Method
cpg	1145.09	J/mol×K	892.42	Joback Method
dvisc	0.0035428	Pa×s	333.97	Joback Method
dvisc	0.0010359	Pa×s	399.17	Joback Method
dvisc	0.0004278	Pa×s	464.38	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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R47269&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume