2-DOCOSANONE

Inchi: InChI=1S/C22H44O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(2)23/h3-
InchiKey: TWBHLKOHVHGYGC-UHFFFAOYSA-N
Formula: C22H44O
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]: 324.59
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.9964		Cheméo Relay (1.0)
gf	5.44	kJ/mol	Joback Method
hf	-634.47	kJ/mol	Cheméo Relay (1.0)
hfus	54.33	kJ/mol	Joback Method
hvap	115.88	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-7.76		Cheméo Relay (1.0)
logp	8.007		Crippen Method
mcvol	322.410	ml/mol	McGowan Method
pc	936.92	kPa	Joback Method
rinpol	389.37		NIST Webbook
rinpol	389.37		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	607.98	K	Cheméo Relay (1.0)
tc	797.42	K	Cheméo Relay (1.0)
tf	340.90	K	Cheméo Relay (1.0)
vc	1.271	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.14	J/mol×K	756.63	Joback Method
cpg	1107.46	J/mol×K	930.05	Joback Method
cpg	1091.28	J/mol×K	901.15	Joback Method

cpg	1074.27	J/mol×K	872.25	Joback Method
cpg	1056.38	J/mol×K	843.34	Joback Method
cpg	1037.59	J/mol×K	814.44	Joback Method
cpg	1017.85	J/mol×K	785.53	Joback Method
dvisc	0.0002260	Pa×s	572.13	Joback Method
dvisc	0.0000737	Pa×s	756.63	Joback Method
dvisc	0.0001003	Pa×s	695.13	Joback Method
dvisc	0.0001447	Pa×s	633.63	Joback Method
dvisc	0.0020125	Pa×s	387.63	Joback Method
dvisc	0.0003931	Pa×s	510.63	Joback Method
dvisc	0.0007953	Pa×s	449.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48436e+01
Coeff. B	-5.50298e+03
Coeff. C	-1.22865e+02
Temperature range (K), min.	500.92
Temperature range (K), max.	700.17

Sources

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=C77327118&Units=SI

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):

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
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