

1,22-Docosanediol

Inchi:	InChI=1S/C22H46O2/c23-21-19-17-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-18-20-22-24
InchiKey:	HIBKFQRBONXURO-UHFFFAOYSA-N
Formula:	C22H46O2
SMILES:	OCCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	342.60
CAS:	22513-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-139.28	kJ/mol	Joback Method
hf	-801.87	kJ/mol	Joback Method
hfus	60.91	kJ/mol	Joback Method
hvap	97.92	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.773		Crippen Method
mcvol	332.580	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
tb	887.12	K	Joback Method
tc	1094.99	K	Joback Method
tf	459.34	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.91	J/molxK	887.12	Joback Method
cpg	1149.46	J/molxK	921.76	Joback Method
cpg	1168.84	J/molxK	956.41	Joback Method
cpg	1187.12	J/molxK	991.05	Joback Method
cpg	1204.37	J/molxK	1025.70	Joback Method
cpg	1220.65	J/molxK	1060.34	Joback Method
cpg	1236.04	J/molxK	1094.99	Joback Method
dvisc	0.0007582	Paxs	459.34	Joback Method
dvisc	0.0001381	Paxs	530.64	Joback Method

dvisc	0.0000377	Paxs	601.93	Joback Method
dvisc	0.0000135	Paxs	673.23	Joback Method
dvisc	0.0000059	Paxs	744.53	Joback Method
dvisc	0.0000030	Paxs	815.82	Joback Method
dvisc	0.0000017	Paxs	887.12	Joback Method
hfust	46.50	kJ/mol	379.40	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22513811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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