Duomeen o

Other names: 1,3-Propanediamine, N-octadecyl-
N-octadecylpropane-1,3-diamine
Inchi: InChI=1S/C21H46N2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-21-18-19-22/h2
InchiKey: DXYUWQFEDOQSQY-UHFFFAOYSA-N
Formula: C21H46N2
SMILES: CCCCCCCCCCCCCCCCCCNCCCN
Mol. weight [g/mol]: 326.60
CAS: 4253-76-3

Physical Properties

Property code	Value	Unit	Source
gf	281.78	kJ/mol	Joback Method
hf	-389.51	kJ/mol	Joback Method
hfus	60.44	kJ/mol	Joback Method
hvap	79.42	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.186		Crippen Method
mcvol	326.710	ml/mol	McGowan Method
pc	998.91	kPa	Joback Method
tb	802.58	K	Joback Method
tc	984.20	K	Joback Method
tf	462.35	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.86	J/mol×K	802.58	Joback Method
cpg	1079.41	J/mol×K	832.85	Joback Method
cpg	1098.94	J/mol×K	863.12	Joback Method
cpg	1117.48	J/mol×K	893.39	Joback Method
cpg	1135.09	J/mol×K	923.66	Joback Method
cpg	1151.80	J/mol×K	953.93	Joback Method
cpg	1167.65	J/mol×K	984.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4253763&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume