Octamylamine

Inchi: InChI=1S/C13H29N/c1-11(2)7-6-8-13(5)14-10-9-12(3)4/h11-14H,6-10H2,1-5H3
InchiKey: RRWTWWBIHKIYTH-UHFFFAOYSA-N
Formula: C13H29N
SMILES: CC(C)CCCC(C)NCCC(C)C
Mol. weight [g/mol]: 199.38
CAS: 502-59-0

Physical Properties

Property code	Value	Unit	Source
gf	140.65	kJ/mol	Joback Method
hf	-274.02	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	49.80	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.837		Crippen Method
mcvol	204.010	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	1303.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1281.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1373.00		NIST Webbook
tb	545.69	K	Joback Method
tc	718.22	K	Joback Method
tf	243.93	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.06	J/mol×K	545.69	Joback Method

cpg	534.62	J/mol×K	574.45	Joback Method
cpg	552.40	J/mol×K	603.20	Joback Method
cpg	569.40	J/mol×K	631.96	Joback Method
cpg	585.66	J/mol×K	660.71	Joback Method
cpg	601.19	J/mol×K	689.47	Joback Method
cpg	616.01	J/mol×K	718.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502590&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume