1-Methyldodecylamine

Other names: 2-Aminotridecane
Inchi: InChI=1S/C13H29N/c1-3-4-5-6-7-8-9-10-11-12-13(2)14/h13H,3-12,14H2,1-2H3
InchiKey: WCLHZVGJULAEJH-UHFFFAOYSA-N
Formula: C13H29N
SMILES: CCCCCCCCCCCC(C)N
Mol. weight [g/mol]: 199.38
CAS: 13205-57-7

Physical Properties

Property code	Value	Unit	Source
gf	122.59	kJ/mol	Joback Method
hf	-283.14	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.255		Crippen Method
mcvol	204.010	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
tb	568.93	K	Joback Method
tc	742.38	K	Joback Method
tf	304.53	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.34	J/mol×K	568.93	Joback Method
cpg	549.04	J/mol×K	597.84	Joback Method
cpg	565.97	J/mol×K	626.75	Joback Method
cpg	582.18	J/mol×K	655.65	Joback Method
cpg	597.66	J/mol×K	684.56	Joback Method
cpg	612.46	J/mol×K	713.47	Joback Method
cpg	626.59	J/mol×K	742.38	Joback Method

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=C13205577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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