1-Dodecanamine, N-methyl-

Other names: N-methyldodecylamine
Inchi: InChI=1S/C13H29N/c1-3-4-5-6-7-8-9-10-11-12-13-14-2/h14H,3-13H2,1-2H3
InchiKey: OMEMQVZNTDHENJ-UHFFFAOYSA-N
Formula: C13H29N
SMILES: CCCCCCCCCCCCNC
Mol. weight [g/mol]: 199.38
CAS: 7311-30-0

Physical Properties

Property code	Value	Unit	Source
gf	147.97	kJ/mol	Joback Method
hf	-258.18	kJ/mol	Joback Method
hfus	34.52	kJ/mol	Joback Method
hvap	50.97	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.127		Crippen Method
mcvol	204.010	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	1486.00		NIST Webbook
tb	547.01	K	Joback Method
tc	710.62	K	Joback Method
tf	291.65 ± 2.00	K	NIST Webbook
tf	291.65 ± 2.00	K	NIST Webbook
tf	289.65 ± 1.50	K	NIST Webbook
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.38	J/mol×K	547.01	Joback Method
cpg	532.82	J/mol×K	574.28	Joback Method
cpg	549.56	J/mol×K	601.55	Joback Method
cpg	565.63	J/mol×K	628.82	Joback Method
cpg	581.04	J/mol×K	656.09	Joback Method

cpg	595.82	J/mol×K	683.35	Joback Method
cpg	609.97	J/mol×K	710.62	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=C7311300&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume