2-Octaneamine, N,N-diethyl

Inchi: InChI=1S/C12H27N/c1-5-8-9-10-11-12(4)13(6-2)7-3/h12H,5-11H2,1-4H3
InchiKey: OFYRDHNOICLKHY-UHFFFAOYSA-N
Formula: C12H27N
SMILES: CCCCCCC(C)N(CC)CC
Mol. weight [g/mol]: 185.35

Physical Properties

Property code	Value	Unit	Source
gf	158.50	kJ/mol	Joback Method
hf	-228.76	kJ/mol	Joback Method
hfus	26.33	kJ/mol	Joback Method
hvap	43.96	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.687		Crippen Method
mcvol	189.920	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1200.00		NIST Webbook
tb	485.96	K	Joback Method
tc	648.86	K	Joback Method
tf	242.47	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.01	J/mol×K	485.96	Joback Method
cpg	459.82	J/mol×K	513.11	Joback Method
cpg	476.90	J/mol×K	540.26	Joback Method
cpg	493.30	J/mol×K	567.41	Joback Method
cpg	509.01	J/mol×K	594.56	Joback Method
cpg	524.07	J/mol×K	621.71	Joback Method
cpg	538.50	J/mol×K	648.86	Joback Method

Sources

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=R540782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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