Diallylaminoacetone

Inchi: InChI=1S/C9H15NO/c1-4-6-10(7-5-2)8-9(3)11/h4-5H,1-2,6-8H2,3H3
InchiKey: NMQNNHLPNMVSQB-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: C=CCN(CC=C)CC(C)=O
Mol. weight [g/mol]: 153.22
CAS: 73813-61-3

Physical Properties

Property code	Value	Unit	Source
gf	182.44	kJ/mol	Joback Method
hf	-23.28	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	43.08	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	1.249		Crippen Method
mcvol	140.620	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	464.99	K	Joback Method
tc	644.30	K	Joback Method
tf	270.07	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.80	J/mol×K	464.99	Joback Method
cpg	309.05	J/mol×K	494.88	Joback Method
cpg	321.65	J/mol×K	524.76	Joback Method
cpg	333.61	J/mol×K	554.65	Joback Method
cpg	344.96	J/mol×K	584.53	Joback Method
cpg	355.72	J/mol×K	614.42	Joback Method
cpg	365.93	J/mol×K	644.30	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=C73813613&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume