

Allylamine, n,n-bis-(2,3-epoxypropyl)-

Inchi:	InChI=1S/C9H15NO2/c1-2-3-10(4-8-6-11-8)5-9-7-12-9/h2,8-9H,1,3-7H2
InchiKey:	QFTYUIDMHYIRNY-UHFFFAOYSA-N
Formula:	C9H15NO2
SMILES:	C=CCN(CC1CO1)CC1CO1
Mol. weight [g/mol]:	169.22
CAS:	49623-99-6

Physical Properties

Property code	Value	Unit	Source
gf	172.78	kJ/mol	Joback Method
hf	-154.53	kJ/mol	Joback Method
hfus	33.03	kJ/mol	Joback Method
hvap	45.85	kJ/mol	Joback Method
log10ws	-0.20		Crippen Method
logp	0.272		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	481.82	K	Joback Method
tc	674.86	K	Joback Method
tf	310.92	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.30	J/molxK	481.82	Joback Method
cpg	339.25	J/molxK	513.99	Joback Method
cpg	354.16	J/molxK	546.17	Joback Method
cpg	368.10	J/molxK	578.34	Joback Method
cpg	381.13	J/molxK	610.51	Joback Method
cpg	393.32	J/molxK	642.68	Joback Method
cpg	404.74	J/molxK	674.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49623996&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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