4-di-n-Butylaminobutanol-1

Inchi: InChI=1S/C12H27NO/c1-3-5-9-13(10-6-4-2)11-7-8-12-14/h14H,3-12H2,1-2H3
InchiKey: WTFHNNKAJBKQSG-UHFFFAOYSA-N
Formula: C12H27NO
SMILES: CCCCN(CCCC)CCCCO
Mol. weight [g/mol]: 201.35
CAS: 41788-34-5

Physical Properties

Property code	Value	Unit	Source
gf	24.12	kJ/mol	Joback Method
hf	-375.71	kJ/mol	Joback Method
hfus	33.94	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.661		Crippen Method
mcvol	195.790	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
tb	578.58	K	Joback Method
tc	735.71	K	Joback Method
tf	318.29	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.94	J/mol×K	578.58	Joback Method
cpg	531.02	J/mol×K	604.77	Joback Method
cpg	545.50	J/mol×K	630.96	Joback Method
cpg	559.37	J/mol×K	657.14	Joback Method
cpg	572.67	J/mol×K	683.33	Joback Method
cpg	585.42	J/mol×K	709.52	Joback Method
cpg	597.62	J/mol×K	735.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41788345&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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