N,N-bis(2-hydroxyethyl)octanamide

Inchi: InChI=1S/C12H25NO3/c1-2-3-4-5-6-7-12(16)13(8-10-14)9-11-15/h14-15H,2-11H2,1H3
InchiKey: FZQAYFWUOCXLKJ-UHFFFAOYSA-N
Formula: C12H25NO3
SMILES: CCCCCCCC(=O)N(CCO)CCO
Mol. weight [g/mol]: 231.33
CAS: 3077-30-3

Physical Properties

Property code	Value	Unit	Source
gf	-241.62	kJ/mol	Joback Method
hf	-640.52	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.160		Crippen Method
mcvol	203.230	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	2024.40		NIST Webbook
rinpol	2024.40		NIST Webbook
tb	724.63	K	Joback Method
tc	893.52	K	Joback Method
tf	429.04	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.65	J/mol×K	724.63	Joback Method
cpg	616.15	J/mol×K	752.78	Joback Method
cpg	628.04	J/mol×K	780.93	Joback Method
cpg	639.36	J/mol×K	809.07	Joback Method
cpg	650.13	J/mol×K	837.22	Joback Method
cpg	660.37	J/mol×K	865.37	Joback Method
cpg	670.11	J/mol×K	893.52	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=C3077303&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

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