Bromoacetamide, N,N-dihexyl-

Inchi: InChI=1S/C14H28BrNO/c1-3-5-7-9-11-16(14(17)13-15)12-10-8-6-4-2/h3-13H2,1-2H3
InchiKey: QAVOJOUQVKLRPP-UHFFFAOYSA-N
Formula: C14H28BrNO
SMILES: CCCCCCN(CCCCCC)C(=O)CBr
Mol. weight [g/mol]: 306.28

Physical Properties

Property code	Value	Unit	Source
gf	63.18	kJ/mol	Joback Method
hf	-351.01	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	61.98	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.371		Crippen Method
mcvol	237.170	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	652.19	K	Joback Method
tc	830.76	K	Joback Method
tf	389.74	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.70	J/mol×K	652.19	Joback Method
cpg	645.18	J/mol×K	681.95	Joback Method
cpg	660.86	J/mol×K	711.71	Joback Method
cpg	675.76	J/mol×K	741.48	Joback Method
cpg	689.92	J/mol×K	771.24	Joback Method
cpg	703.37	J/mol×K	801.00	Joback Method
cpg	716.15	J/mol×K	830.76	Joback Method

Sources

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=U308169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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