Bromacetamide, N-undecyl-

Inchi: InChI=1S/C13H26BrNO/c1-2-3-4-5-6-7-8-9-10-11-15-13(16)12-14/h2-12H2,1H3,(H,15,16
InchiKey: IQFUCUSYPRBRFH-UHFFFAOYSA-N
Formula: C13H26BrNO
SMILES: CCCCCCCCCCCNC(=O)CBr
Mol. weight [g/mol]: 292.26

Physical Properties

Property code	Value	Unit	Source
gf	33.37	kJ/mol	Joback Method
hf	-344.43	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.028		Crippen Method
mcvol	223.080	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	667.04	K	Joback Method
tc	850.26	K	Joback Method
tf	398.66	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.38	J/mol×K	667.04	Joback Method
cpg	608.79	J/mol×K	697.58	Joback Method
cpg	623.43	J/mol×K	728.11	Joback Method
cpg	637.34	J/mol×K	758.65	Joback Method
cpg	650.54	J/mol×K	789.19	Joback Method
cpg	663.08	J/mol×K	819.72	Joback Method
cpg	674.97	J/mol×K	850.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407080&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
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