Bromoacetamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C17H34BrNO/c1-3-5-7-9-11-13-15-19(17(20)16-18)14-12-10-8-6-4-2/h3-16H2,
InchiKey: QLRLBCAQISQMGS-UHFFFAOYSA-N
Formula: C17H34BrNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)CBr
Mol. weight [g/mol]: 348.36

Physical Properties

Property code	Value	Unit	Source
gf	88.44	kJ/mol	Joback Method
hf	-412.93	kJ/mol	Joback Method
hfus	49.69	kJ/mol	Joback Method
hvap	68.66	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.541		Crippen Method
mcvol	279.440	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	720.83	K	Joback Method
tc	898.74	K	Joback Method
tf	423.55	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.79	J/mol×K	720.83	Joback Method
cpg	814.46	J/mol×K	750.48	Joback Method
cpg	831.25	J/mol×K	780.13	Joback Method
cpg	847.22	J/mol×K	809.79	Joback Method
cpg	862.39	J/mol×K	839.44	Joback Method
cpg	876.81	J/mol×K	869.09	Joback Method
cpg	890.52	J/mol×K	898.74	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=U308172&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