Bromacetamide, N-nonyl-

Inchi: InChI=1S/C11H22BrNO/c1-2-3-4-5-6-7-8-9-13-11(14)10-12/h2-10H2,1H3,(H,13,14)
InchiKey: XFFLALILCICPPR-UHFFFAOYSA-N
Formula: C11H22BrNO
SMILES: CCCCCCCCCNC(=O)CBr
Mol. weight [g/mol]: 264.20

Physical Properties

Property code	Value	Unit	Source
gf	16.53	kJ/mol	Joback Method
hf	-303.15	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.248		Crippen Method
mcvol	194.900	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
tb	621.28	K	Joback Method
tc	807.38	K	Joback Method
tf	376.12	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.86	J/mol×K	621.28	Joback Method
cpg	503.23	J/mol×K	652.30	Joback Method
cpg	516.89	J/mol×K	683.31	Joback Method
cpg	529.85	J/mol×K	714.33	Joback Method
cpg	542.16	J/mol×K	745.35	Joback Method
cpg	553.83	J/mol×K	776.36	Joback Method
cpg	564.90	J/mol×K	807.38	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=U407078&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

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