Bromacetamide, N-(hept-2-yl)-

Inchi: InChI=1S/C9H18BrNO/c1-3-4-5-6-8(2)11-9(12)7-10/h8H,3-7H2,1-2H3,(H,11,12)
InchiKey: AQZMQRAZXBVCRO-UHFFFAOYSA-N
Formula: C9H18BrNO
SMILES: CCCCCC(C)N=C(O)CBr
Mol. weight [g/mol]: 236.15

Physical Properties

Property code	Value	Unit	Source
hf	-287.84	kJ/mol	Joback Method
hvap	61.75	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.307		Crippen Method
mcvol	166.720	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook
tb	639.78	K	Joback Method
tc	832.04	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407074&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation 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