

Bromacetamide, N-(2-ethylhexyl)-

Inchi:	InChI=1S/C10H20BrNO/c1-3-5-6-9(4-2)8-12-10(13)7-11/h9H,3-8H2,1-2H3,(H,12,13)
InchiKey:	FTYPZJUOXZNGDV-UHFFFAOYSA-N
Formula:	C10H20BrNO
SMILES:	CCCCC(CC)CN=C(O)CBr
Mol. weight [g/mol]:	250.18

Physical Properties

Property code	Value	Unit	Source
hf	-308.48	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.554		Crippen Method
mcvol	180.810	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	662.66	K	Joback Method
tc	853.01	K	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=U407075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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