

5-Bromovaleric acid, nonyl ester

Inchi:	InChI=1S/C14H27BrO2/c1-2-3-4-5-6-7-10-13-17-14(16)11-8-9-12-15/h2-13H2,1H3
InchiKey:	ZZYSKZVWOPSDZ-UHFFFAOYSA-N
Formula:	C14H27BrO2
SMILES:	CCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]:	307.27

Physical Properties

Property code	Value	Unit	Source
gf	-152.60	kJ/mol	Joback Method
hf	-550.76	kJ/mol	Joback Method
hfus	40.09	kJ/mol	Joback Method
hvap	62.35	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.845		Crippen Method
mvol	233.060	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	662.17	K	Joback Method
tc	841.70	K	Joback Method
tf	379.50	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.88	J/molxK	662.17	Joback Method
cpg	690.40	J/molxK	811.78	Joback Method
cpg	677.31	J/molxK	781.86	Joback Method
cpg	663.54	J/molxK	751.94	Joback Method
cpg	649.05	J/molxK	722.01	Joback Method
cpg	633.84	J/molxK	692.09	Joback Method
cpg	702.81	J/molxK	841.70	Joback Method
dvisc	0.0001351	Paxs	662.17	Joback Method

dvisc	0.0001759	Paxs	615.06	Joback Method
dvisc	0.0002393	Paxs	567.95	Joback Method
dvisc	0.0003442	Paxs	520.84	Joback Method
dvisc	0.0005321	Paxs	473.72	Joback Method
dvisc	0.0009057	Paxs	426.61	Joback Method
dvisc	0.0017594	Paxs	379.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U299980&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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