

5-Bromovaleric acid, decyl ester

Inchi:	InChI=1S/C15H29BrO2/c1-2-3-4-5-6-7-8-11-14-18-15(17)12-9-10-13-16/h2-14H2,1H3
InchiKey:	GHTHELFDXOZRSL-UHFFFAOYSA-N
Formula:	C15H29BrO2
SMILES:	CCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]:	321.29
CAS:	175083-30-4

Physical Properties

Property code	Value	Unit	Source
gf	-144.18	kJ/mol	Joback Method
hf	-571.40	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	64.58	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.236		Crippen Method
mvol	247.150	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	1935.80		NIST Webbook
tb	685.05	K	Joback Method
tc	863.97	K	Joback Method
tf	390.77	K	Joback Method
vc	0.962	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.62	J/molxK	685.05	Joback Method
cpg	689.04	J/molxK	714.87	Joback Method
cpg	704.68	J/molxK	744.69	Joback Method
cpg	719.56	J/molxK	774.51	Joback Method
cpg	733.70	J/molxK	804.33	Joback Method
cpg	747.13	J/molxK	834.15	Joback Method
cpg	759.87	J/molxK	863.97	Joback Method
dvisc	0.0016131	Paxs	390.77	Joback Method

dvisc	0.0008189	Paxs	439.82	Joback Method
dvisc	0.0004762	Paxs	488.86	Joback Method
dvisc	0.0003058	Paxs	537.91	Joback Method
dvisc	0.0002114	Paxs	586.96	Joback Method
dvisc	0.0001547	Paxs	636.00	Joback Method
dvisc	0.0001184	Paxs	685.05	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=C175083304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

Latest version available from:

<https://www.chemeo.com/cid/51-765-6/5-Bromovaleric-acid-decyl-ester.pdf>

Generated by Cheméo on 2024-04-19 16:44:02.938025727 +0000 UTC m=+15834291.858603043.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.