

4-Bromobutanoic acid, undec-2-enyl ester

Inchi:	InChI=1S/C15H27BrO2/c1-2-3-4-5-6-7-8-9-10-14-18-15(17)12-11-13-16/h9-10H,2-8,11-14
InchiKey:	QBCPDDNDBOJMNN-MDZDMXLPSA-N
Formula:	C15H27BrO2
SMILES:	CCCCCCCCC=CCOC(=O)CCCB
Mol. weight [g/mol]:	319.28

Physical Properties

Property code	Value	Unit	Source
gf	-63.96	kJ/mol	Joback Method
hf	-454.18	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	5.011		Crippen Method
mvol	242.850	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	689.21	K	Joback Method
tc	873.47	K	Joback Method
tf	385.69	K	Joback Method
vc	0.942	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.27	J/molxK	689.21	Joback Method
cpg	722.41	J/molxK	842.76	Joback Method
cpg	709.43	J/molxK	812.05	Joback Method
cpg	695.76	J/molxK	781.34	Joback Method
cpg	681.36	J/molxK	750.63	Joback Method
cpg	666.21	J/molxK	719.92	Joback Method
cpg	734.72	J/molxK	873.47	Joback Method
dvisc	0.0001021	Paxs	689.21	Joback Method

dvisc	0.0001339	Paxs	638.62	Joback Method
dvisc	0.0001838	Paxs	588.04	Joback Method
dvisc	0.0002678	Paxs	537.45	Joback Method
dvisc	0.0004219	Paxs	486.86	Joback Method
dvisc	0.0007388	Paxs	436.28	Joback Method
dvisc	0.0014983	Paxs	385.69	Joback Method

Sources

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=U299283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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