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,2-8,11-1
InchiKey: QBCPDDNDBOJMNN-MDZDMXLPSA-N
Formula: C15H27BrO2
SMILES: CCCCCCCCC=CCOC(=O)CCCBr
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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001339	Pa×s	638.62	Joback Method
dvisc	0.0001838	Pa×s	588.04	Joback Method
dvisc	0.0002678	Pa×s	537.45	Joback Method
dvisc	0.0004219	Pa×s	486.86	Joback Method
dvisc	0.0007388	Pa×s	436.28	Joback Method
dvisc	0.0014983	Pa×s	385.69	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=U299283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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