6-Bromohexanoic acid, undec-2-enyl ester

Inchi: InChI=1S/C17H31BrO2/c1-2-3-4-5-6-7-8-9-13-16-20-17(19)14-11-10-12-15-18/h9,13H,2-
InchiKey: FXIDHPHTLPRIER-UKTHLTGXSA-N
Formula: C17H31BrO2
SMILES: CCCCCCCCC=CCOC(=O)CCCCCBr
Mol. weight [g/mol]: 347.33

Physical Properties

Property code	Value	Unit	Source
gf	-47.12	kJ/mol	Joback Method
hf	-495.46	kJ/mol	Joback Method
hfus	48.06	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.792		Crippen Method
mcvol	271.030	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	734.97	K	Joback Method
tc	918.46	K	Joback Method
tf	408.23	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.24	J/mol×K	734.97	Joback Method
cpg	838.05	J/mol×K	887.88	Joback Method
cpg	824.42	J/mol×K	857.30	Joback Method
cpg	810.06	J/mol×K	826.72	Joback Method
cpg	794.93	J/mol×K	796.13	Joback Method
cpg	779.00	J/mol×K	765.55	Joback Method
cpg	850.99	J/mol×K	918.46	Joback Method
dvisc	0.0000780	Pa×s	734.97	Joback Method

dvisc	0.0001028	Pa×s	680.51	Joback Method
dvisc	0.0001423	Pa×s	626.06	Joback Method
dvisc	0.0002094	Pa×s	571.60	Joback Method
dvisc	0.0003344	Pa×s	517.14	Joback Method
dvisc	0.0005961	Pa×s	462.69	Joback Method
dvisc	0.0012401	Pa×s	408.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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