4-Bromobutanoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C12H21BrO2/c1-3-4-5-6-8-11(2)15-12(14)9-7-10-13/h6,8,11H,3-5,7,9-10H2,1-
InchiKey: YGSZKEKARQJBAA-SOFGYWHQSA-N
Formula: C12H21BrO2
SMILES: CCCCC=CC(C)OC(=O)CCCBr
Mol. weight [g/mol]: 277.20

Physical Properties

Property code	Value	Unit	Source
gf	-91.66	kJ/mol	Joback Method
hf	-397.54	kJ/mol	Joback Method
hfus	31.59	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.840		Crippen Method
mcvol	200.580	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1590.00		NIST Webbook
tb	620.13	K	Joback Method
tc	812.08	K	Joback Method
tf	336.88	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.24	J/mol×K	620.13	Joback Method
cpg	506.98	J/mol×K	652.12	Joback Method
cpg	520.96	J/mol×K	684.11	Joback Method
cpg	534.22	J/mol×K	716.11	Joback Method
cpg	546.80	J/mol×K	748.10	Joback Method
cpg	558.71	J/mol×K	780.09	Joback Method
cpg	569.98	J/mol×K	812.08	Joback Method
dvisc	0.0024191	Pa×s	336.88	Joback Method
dvisc	0.0011213	Pa×s	384.09	Joback Method

dvisc	0.0006150	Pa×s	431.30	Joback Method
dvisc	0.0003798	Pa×s	478.50	Joback Method
dvisc	0.0002557	Pa×s	525.71	Joback Method
dvisc	0.0001838	Pa×s	572.92	Joback Method
dvisc	0.0001389	Pa×s	620.13	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=U299279&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