5-bromovaleric acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C13H23BrO2/c1-3-4-5-6-9-12(2)16-13(15)10-7-8-11-14/h6,9,12H,3-5,7-8,10-11

InchiKey: PIOWGKOAQGEQCT-RMKNXTFCSA-N

Formula: C13H23BrO2

SMILES: CCCC/C=C/C(C)OC(=O)CCCCBr

Mol. weight [g/mol]: 291.23

Physical Properties

Property code	Value	Unit	Source
hf	-549.57	kJ/mol	Cheméo Relay (1.0)
hfus	34.18	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Cheméo Relay (1.0)
logp	4.230		Crippen Method
mcvol	214.670	ml/mol	McGowan Method
rinpol	1744.60		NIST Webbook
rinpol	1744.60		NIST Webbook
tb	536.40	K	Cheméo Relay (1.0)
tc	720.17	K	Cheméo Relay (1.0)
tf	242.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.70	J/mol×K	643.01	Joback Method
cpg	558.98	J/mol×K	674.66	Joback Method
cpg	573.49	J/mol×K	706.32	Joback Method
cpg	587.24	J/mol×K	737.97	Joback Method
cpg	600.29	J/mol×K	769.62	Joback Method
cpg	612.65	J/mol×K	801.27	Joback Method
cpg	624.35	J/mol×K	832.93	Joback Method
dvisc	0.0022293	Pa×s	348.15	Joback Method
dvisc	0.0010197	Pa×s	397.29	Joback Method
dvisc	0.0005540	Pa×s	446.44	Joback Method
dvisc	0.0003397	Pa×s	495.58	Joback Method
dvisc	0.0002276	Pa×s	544.72	Joback Method

dvisc	0.0001629	Pa×s	593.87	Joback Method
dvisc	0.0001227	Pa×s	643.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292566&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point