5-bromovaleric acid, octyl ester

Inchi: InChI=1S/C13H25BrO2/c1-2-3-4-5-6-9-12-16-13(15)10-7-8-11-14/h2-12H2,1H3
InchiKey: WJGKHCBEUVDHNP-UHFFFAOYSA-N
Formula: C13H25BrO2
SMILES: CCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 293.24

Physical Properties

Property code	Value	Unit	Source
af	0.8190		Cheméo Relay (1.0)
hf	-621.36	kJ/mol	Cheméo Relay (1.0)
hfus	37.50	kJ/mol	Joback Method
hvap	77.60	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	Cheméo Relay (1.0)
log10ws	-4.83		Cheméo Relay (1.0)
logp	4.455		Crippen Method
mcvol	218.970	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1823.00		NIST Webbook
tb	574.61	K	Cheméo Relay (1.0)
tc	745.01	K	Cheméo Relay (1.0)
tf	266.16	K	Cheméo Relay (1.0)
vc	0.819	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.45	J/mol×K	639.29	Joback Method
cpg	579.92	J/mol×K	669.38	Joback Method
cpg	594.66	J/mol×K	699.47	Joback Method
cpg	608.71	J/mol×K	729.56	Joback Method
cpg	622.07	J/mol×K	759.65	Joback Method
cpg	634.77	J/mol×K	789.74	Joback Method
cpg	646.83	J/mol×K	819.82	Joback Method
dvisc	0.0019071	Pa×s	368.23	Joback Method

dvisc	0.0009964	Pa×s	413.41	Joback Method
dvisc	0.0005916	Pa×s	458.58	Joback Method
dvisc	0.0003857	Pa×s	503.76	Joback Method
dvisc	0.0002698	Pa×s	548.94	Joback Method
dvisc	0.0001993	Pa×s	594.11	Joback Method
dvisc	0.0001536	Pa×s	639.29	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=C13931447&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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