5-Bromovaleric acid, 2-adamantyl ester

Inchi: InChI=1S/C15H23BrO2/c16-4-2-1-3-14(17)18-15-12-6-10-5-11(8-12)9-13(15)7-10/h10-13
InchiKey: FVVKQQWMMIYVEM-UHFFFAOYSA-N
Formula: C15H23BrO2
SMILES: O=C(CCCCBr)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 315.25

Physical Properties

Property code	Value	Unit	Source
gf	10.55	kJ/mol	Joback Method
hf	-399.84	kJ/mol	Joback Method
hfus	37.12	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.919		Crippen Method
mcvol	214.570	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	2108.00		NIST Webbook
tb	700.20	K	Joback Method
tc	915.40	K	Joback Method
tf	432.59	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.06	J/mol×K	700.20	Joback Method
cpg	719.92	J/mol×K	879.53	Joback Method
cpg	705.16	J/mol×K	843.67	Joback Method
cpg	689.49	J/mol×K	807.80	Joback Method
cpg	672.81	J/mol×K	771.93	Joback Method
cpg	655.04	J/mol×K	736.07	Joback Method
cpg	733.86	J/mol×K	915.40	Joback Method
dvisc	0.0025458	Pa×s	700.20	Joback Method
dvisc	0.0026846	Pa×s	655.60	Joback Method

dvisc	0.0028529	Pa×s	611.00	Joback Method
dvisc	0.0030611	Pa×s	566.39	Joback Method
dvisc	0.0033242	Pa×s	521.79	Joback Method
dvisc	0.0036660	Pa×s	477.19	Joback Method
dvisc	0.0041253	Pa×s	432.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299981&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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