5-Bromovaleric acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C17H27BrO2/c18-5-2-1-3-16(19)20-6-4-17-10-13-7-14(11-17)9-15(8-13)12-17/

InchiKey: DWFTVALNRLUJIW-UHFFFAOYSA-N

Formula: C17H27BrO2

SMILES: O=C(CCCCBr)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 343.30

Physical Properties

Property code	Value	Unit	Source
gf	29.61	kJ/mol	Joback Method
hf	-405.54	kJ/mol	Joback Method
hfus	34.94	kJ/mol	Joback Method
hvap	67.48	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.701		Crippen Method
mcvol	242.750	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2354.00		NIST Webbook
rinpol	2354.00		NIST Webbook
tb	750.87	K	Joback Method
tc	966.71	K	Joback Method
tf	483.27	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.82	J/mol×K	750.87	Joback Method
cpg	761.26	J/mol×K	786.84	Joback Method
cpg	779.96	J/mol×K	822.82	Joback Method
cpg	798.12	J/mol×K	858.79	Joback Method
cpg	815.95	J/mol×K	894.76	Joback Method
cpg	833.62	J/mol×K	930.74	Joback Method
cpg	851.34	J/mol×K	966.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299983&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
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