4-Bromobutyric acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C9H17BrO2/c1-7(2)8(3)12-9(11)5-4-6-10/h7-8H,4-6H2,1-3H3
InchiKey: YRPLOBCIKDOYHQ-UHFFFAOYSA-N
Formula: C9H17BrO2
SMILES: CC(C)C(C)OC(=O)CCCBr
Mol. weight [g/mol]: 237.13

Physical Properties

Property code	Value	Unit	Source
gf	-199.58	kJ/mol	Joback Method
hf	-458.12	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.749		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
tb	546.89	K	Joback Method
tc	742.11	K	Joback Method
tf	293.15	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.43	J/mol×K	546.89	Joback Method
cpg	427.46	J/mol×K	709.57	Joback Method
cpg	416.48	J/mol×K	677.03	Joback Method
cpg	404.89	J/mol×K	644.50	Joback Method
cpg	392.70	J/mol×K	611.96	Joback Method
cpg	379.88	J/mol×K	579.43	Joback Method
cpg	437.87	J/mol×K	742.11	Joback Method
dvisc	0.0002165	Pa×s	546.89	Joback Method

dvisc	0.0002891	Pa×s	504.60	Joback Method
dvisc	0.0004070	Pa×s	462.31	Joback Method
dvisc	0.0006139	Pa×s	420.02	Joback Method
dvisc	0.0010150	Pa×s	377.73	Joback Method
dvisc	0.0019052	Pa×s	335.44	Joback Method
dvisc	0.0042885	Pa×s	293.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354683&Units=SI

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