4-Bromobutanoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C9H15BrO2/c1-8(2)5-7-12-9(11)4-3-6-10/h5H,3-4,6-7H2,1-2H3
InchiKey: PKKFLEBSMPTFBK-UHFFFAOYSA-N
Formula: C9H15BrO2
SMILES: CC(C)=CCOC(=O)CCCBr
Mol. weight [g/mol]: 235.12

Physical Properties

Property code	Value	Unit	Source
gf	-123.03	kJ/mol	Joback Method
hf	-340.13	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	51.26	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.671		Crippen Method
mcvol	158.310	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
tb	551.81	K	Joback Method
tc	750.75	K	Joback Method
tf	304.11	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.62	J/mol×K	551.81	Joback Method
cpg	359.10	J/mol×K	584.97	Joback Method
cpg	370.95	J/mol×K	618.12	Joback Method
cpg	382.17	J/mol×K	651.28	Joback Method
cpg	392.81	J/mol×K	684.44	Joback Method
cpg	402.88	J/mol×K	717.59	Joback Method
cpg	412.42	J/mol×K	750.75	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=U299276&Units=SI

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

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