2-Ethylbutyric acid, 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C9H14BrF3O2/c1-3-6(4-2)8(14)15-7(5-10)9(11,12)13/h6-7H,3-5H2,1-2H3

InchiKey: UABXDKCZFCHYFO-UHFFFAOYSA-N

Formula: C9H14BrF3O2

SMILES: CCC(CC)C(=O)OC(CBr)C(F)(F)F

Mol. weight [g/mol]: 291.11

Physical Properties

Property code	Value	Unit	Source
gf	-781.17	kJ/mol	Joback Method
hf	-1055.20	kJ/mol	Joback Method
hfus	21.92	kJ/mol	Joback Method
hvap	46.70	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.292		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1056.00		NIST Webbook
tb	541.47	K	Joback Method
tc	721.08	K	Joback Method
tf	297.34	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.49	J/mol×K	541.47	Joback Method
cpg	406.92	J/mol×K	571.41	Joback Method
cpg	418.68	J/mol×K	601.34	Joback Method
cpg	429.80	J/mol×K	631.28	Joback Method
cpg	440.31	J/mol×K	661.21	Joback Method
cpg	450.23	J/mol×K	691.15	Joback Method
cpg	459.58	J/mol×K	721.08	Joback Method

Sources

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=U370813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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