Acetic acid, trifluoro-, 1,2-dimethylbutyl ester, (R*,S*)-(+/-)-

Inchi: InChI=1S/C8H13F3O2/c1-4-5(2)6(3)13-7(12)8(9,10)11/h5-6H,4H2,1-3H3
InchiKey: SSJZIAKRAUGSQG-UHFFFAOYSA-N
Formula: C8H13F3O2
SMILES: CCC(C)C(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 198.18
CAS: 74454-47-0

Physical Properties

Property code	Value	Unit	Source
gf	-803.91	kJ/mol	Joback Method
hf	-1060.89	kJ/mol	Joback Method
hfus	14.04	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.526		Crippen Method
mcvol	136.330	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	452.43	K	Joback Method
tc	619.30	K	Joback Method
tf	226.27	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.29	J/mol×K	452.43	Joback Method
cpg	319.56	J/mol×K	480.24	Joback Method
cpg	331.29	J/mol×K	508.05	Joback Method
cpg	342.48	J/mol×K	535.87	Joback Method
cpg	353.15	J/mol×K	563.68	Joback Method
cpg	363.32	J/mol×K	591.49	Joback Method
cpg	372.99	J/mol×K	619.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74454470&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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