Bis(2,2,2-trifluoroethyl) itaconate

Inchi: InChI=1S/C9H8F6O4/c1-5(7(17)19-4-9(13,14)15)2-6(16)18-3-8(10,11)12/h1-4H2
InchiKey: IRXUFAGEXMCXHZ-UHFFFAOYSA-N
Formula: C9H8F6O4
SMILES: C=C(CC(=O)OCC(F)(F)F)C(=O)OCC(F)(F)F
Mol. weight [g/mol]: 294.15
CAS: 104534-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-1526.83	kJ/mol	Joback Method
hf	-1797.21	kJ/mol	Joback Method
hfus	25.70	kJ/mol	Joback Method
hvap	45.86	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.144		Crippen Method
mcvol	158.870	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
tb	543.62	K	Joback Method
tc	704.76	K	Joback Method
tf	328.17	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.80	J/mol×K	543.62	Joback Method
cpg	415.05	J/mol×K	570.48	Joback Method
cpg	424.74	J/mol×K	597.33	Joback Method
cpg	433.88	J/mol×K	624.19	Joback Method
cpg	442.49	J/mol×K	651.05	Joback Method
cpg	450.60	J/mol×K	677.91	Joback Method
cpg	458.22	J/mol×K	704.76	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=C104534965&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume