Propionic acid, 2,2-dichloro-3,3,3-trifluoro-, methyl ester

Inchi: InChI=1S/C4H3Cl2F3O2/c1-11-2(10)3(5,6)4(7,8)9/h1H3
InchiKey: CXTHLUIZHFAWKT-UHFFFAOYSA-N
Formula: C4H3Cl2F3O2
SMILES: COC(=O)C(Cl)(Cl)C(F)(F)F
Mol. weight [g/mol]: 210.97
CAS: 378-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-853.73	kJ/mol	Joback Method
hf	-1008.00	kJ/mol	Joback Method
hfus	11.71	kJ/mol	Joback Method
hvap	37.38	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.896		Crippen Method
mcvol	104.450	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	433.42	K	Joback Method
tc	621.69	K	Joback Method
tf	273.45	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.15	J/mol×K	433.42	Joback Method
cpg	210.60	J/mol×K	464.80	Joback Method
cpg	217.50	J/mol×K	496.18	Joback Method
cpg	223.85	J/mol×K	527.56	Joback Method
cpg	229.70	J/mol×K	558.94	Joback Method
cpg	235.07	J/mol×K	590.32	Joback Method
cpg	239.98	J/mol×K	621.69	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=C378687&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume