Methyl pentafluoropropionylacetate

Inchi: InChI=1S/C6H5F5O3/c1-14-4(13)2-3(12)5(7,8)6(9,10)11/h2H2,1H3
InchiKey: FGGMNRZYEBHEIR-UHFFFAOYSA-N
Formula: C6H5F5O3
SMILES: COC(=O)CC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 220.09
CAS: 104857-88-7

Physical Properties

Property code	Value	Unit	Source
gf	-1331.57	kJ/mol	Joback Method
hf	-1522.60	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	38.17	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.316		Crippen Method
mcvol	113.260	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	456.73	K	Joback Method
tc	622.27	K	Joback Method
tf	287.26	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.87	J/mol×K	456.73	Joback Method
cpg	271.85	J/mol×K	484.32	Joback Method
cpg	280.29	J/mol×K	511.91	Joback Method
cpg	288.23	J/mol×K	539.50	Joback Method
cpg	295.67	J/mol×K	567.09	Joback Method
cpg	302.64	J/mol×K	594.68	Joback Method
cpg	309.16	J/mol×K	622.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104857887&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

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