Ethyl pentafluoropropionylacetate

Other names: Ethyl pentafluoropropionylacetate
Inchi: InChI=1S/C7H7F5O3/c1-2-15-5(14)3-4(13)6(8,9)7(10,11)12/h2-3H2,1H3
InchiKey: MWGSZQXKIYWSFS-UHFFFAOYSA-N
Formula: C7H7F5O3
SMILES: CCOC(=O)CC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 234.12

Physical Properties

Property code	Value	Unit	Source
af	0.4571		Cheméo Relay (1.0)
gf	-1323.15	kJ/mol	Joback Method
hf	-1668.12	kJ/mol	Cheméo Relay (1.0)
hfus	18.84	kJ/mol	Joback Method
hvap	50.34	kJ/mol	Cheméo Relay (1.0)
ie	10.40	eV	Cheméo Relay (1.0)
log10ws	-2.30		Cheméo Relay (1.0)
logp	1.706		Crippen Method
mcvol	127.350	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	401.74	K	Cheméo Relay (1.0)
tc	537.95	K	Cheméo Relay (1.0)
tf	240.65	K	Cheméo Relay (1.0)
vc	0.456	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.81	J/mol×K	479.61	Joback Method
cpg	313.67	J/mol×K	507.04	Joback Method
cpg	322.96	J/mol×K	534.47	Joback Method
cpg	331.72	J/mol×K	561.91	Joback Method
cpg	339.95	J/mol×K	589.34	Joback Method
cpg	347.68	J/mol×K	616.77	Joback Method
cpg	354.94	J/mol×K	644.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C663354&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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