Ethyl heptafluorobutanoylacetate

Other names: Ethyl heptafluorobutyrylacetate
Inchi: InChI=1S/C8H7F7O3/c1-2-18-5(17)3-4(16)6(9,10)7(11,12)8(13,14)15/h2-3H2,1H3
InchiKey: CMGCMFZWEPCGSQ-UHFFFAOYSA-N
Formula: C8H7F7O3
SMILES: CCOC(=O)CC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 284.13
CAS: 336-62-9

Physical Properties

Property code	Value	Unit	Source
gf	-1701.51	kJ/mol	Joback Method
hf	-1964.85	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	39.70	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.342		Crippen Method
mcvol	144.980	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
tb	497.80	K	Joback Method
tc	655.68	K	Joback Method
tf	313.40	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.41	J/mol×K	497.80	Joback Method
cpg	376.94	J/mol×K	524.11	Joback Method
cpg	386.81	J/mol×K	550.43	Joback Method
cpg	396.06	J/mol×K	576.74	Joback Method
cpg	404.71	J/mol×K	603.06	Joback Method
cpg	412.78	J/mol×K	629.37	Joback Method
cpg	420.32	J/mol×K	655.68	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=C336629&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