2,4-Hexanedione, 1,1,1-trifluoro-5,5-dimethyl-

Other names: 1,1,1-Trifluoro-5,5-dimethyl-2,4-hexanedione
1,1,1-trifluoro-5,5-dimethylhexane-2,4-dione
Inchi: InChI=1S/C8H11F3O2/c1-7(2,3)5(12)4-6(13)8(9,10)11/h4H2,1-3H3
InchiKey: BVPKYBMUQDZTJH-UHFFFAOYSA-N
Formula: C8H11F3O2
SMILES: CC(C)(C)C(=O)CC(=O)C(F)(F)F
Mol. weight [g/mol]: 196.17
CAS: 22767-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-820.11	kJ/mol	Joback Method
hf	-1039.44	kJ/mol	Joback Method
hfus	14.09	kJ/mol	Joback Method
hvap	41.85	kJ/mol	Joback Method
ie	9.87 ± 0.07	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.123		Crippen Method
mcvol	132.030	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	481.53	K	Joback Method
tc	661.77	K	Joback Method
tf	286.39	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.21	J/mol×K	481.53	Joback Method
cpg	318.25	J/mol×K	511.57	Joback Method
cpg	329.54	J/mol×K	541.61	Joback Method
cpg	340.11	J/mol×K	571.65	Joback Method
cpg	350.00	J/mol×K	601.69	Joback Method
cpg	359.23	J/mol×K	631.73	Joback Method

cpg	367.87	J/mol×K	661.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.50 ± 1.50	K	0.80	NIST Webbook

Sources

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=C22767904&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume