3,5-Octanedione, 6,6,7,7,8,8,8-heptafluoro-2,2-dimethyl-

Other names: 1,1,1,2,2,3,3-Heptafluoro-7,7-dimethyl-4,6-octanedione
2,2-Dimethyl-6,6,7,7,8,8,8-heptafluoro-3,5-octanedione
6,6,7,7,8,8,8-Heptafluoro-2,2-dimethyl-3,5-octanedione
6,6,7,7,8,8,8-heptafluoro-2,2-dimethyloctane-3,5-dione

Inchi: InChI=1S/C10H11F7O2/c1-7(2,3)5(18)4-6(19)8(11,12)9(13,14)10(15,16)17/h4H2,1-3H3

InchiKey: SQNZLBOJCWQLGQ-UHFFFAOYSA-N

Formula: C10H11F7O2

SMILES: CC(C)(C)C(=O)CC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 296.18

CAS: 17587-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-1576.83	kJ/mol	Joback Method
hf	-1882.66	kJ/mol	Joback Method
hfus	16.76	kJ/mol	Joback Method
hvap	40.44	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.394		Crippen Method
mcvol	167.290	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
tb	517.91	K	Joback Method
tc	682.52	K	Joback Method
tf	316.13	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.90	J/mol×K	517.91	Joback Method
cpg	447.82	J/mol×K	545.34	Joback Method
cpg	459.83	J/mol×K	572.78	Joback Method
cpg	470.98	J/mol×K	600.21	Joback Method
cpg	481.33	J/mol×K	627.65	Joback Method

cpg	490.92	J/mol×K	655.08	Joback Method
cpg	499.81	J/mol×K	682.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	319.50 ± 0.50	K	0.70	NIST Webbook
tbrp	319.70	K	0.70	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=C17587223&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
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