1,1,1,5,5,6,6,6-Octafluoro-2,4-hexanedione

Inchi: InChI=1S/C6H2F8O2/c7-4(8,6(12,13)14)2(15)1-3(16)5(9,10)11/h1H2
InchiKey: MGKBKOFWQWACLM-UHFFFAOYSA-N
Formula: C6H2F8O2
SMILES: O=C(CC(=O)C(F)(F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 258.07
CAS: 20825-07-4

Physical Properties

Property code	Value	Unit	Source
gf	-1808.16	kJ/mol	Joback Method
hf	-1987.46	kJ/mol	Joback Method
hfus	16.89	kJ/mol	Joback Method
hvap	32.02	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.275		Crippen Method
mcvol	112.700	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	428.89	K	Joback Method
tc	580.26	K	Joback Method
tf	269.22	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.04	J/mol×K	428.89	Joback Method
cpg	277.16	J/mol×K	454.12	Joback Method
cpg	285.65	J/mol×K	479.35	Joback Method
cpg	293.52	J/mol×K	504.58	Joback Method
cpg	300.82	J/mol×K	529.80	Joback Method
cpg	307.57	J/mol×K	555.03	Joback Method
cpg	313.81	J/mol×K	580.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20825074&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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