cis-Dimethyl perfluoro(4-methyl-2-pentene)dioate

Inchi: InChI=1S/C8H6F6O4/c1-17-5(15)3(9)4(10)7(11,6(16)18-2)8(12,13)14/h1-2H3/b4-3-

InchiKey: BWKRYZOYJDOWHI-ARJAWSKDSA-N

Formula: C8H6F6O4

SMILES: COC(=O)C(F)=C(F)C(F)(C(=O)OC)C(F)(F)F

Mol. weight [g/mol]: 280.12

CAS: 74032-60-3

Physical Properties

Property code	Value	Unit	Source
gf	-1551.42	kJ/mol	Joback Method
hf	-1794.57	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.754		Crippen Method
mcvol	144.780	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
tb	528.10	K	Joback Method
tc	696.17	K	Joback Method
tf	299.62	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.04	J/mol×K	528.10	Joback Method
cpg	369.75	J/mol×K	556.11	Joback Method
cpg	378.87	J/mol×K	584.12	Joback Method
cpg	387.43	J/mol×K	612.13	Joback Method
cpg	395.45	J/mol×K	640.15	Joback Method
cpg	402.96	J/mol×K	668.16	Joback Method
cpg	409.98	J/mol×K	696.17	Joback Method

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=C74032603&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume