Diethylmalonic acid, monochloride, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H13ClF8O3/c1-3-9(4-2,6(13)22)8(23)24-5-10(16,17)12(20,21)11(18,19)7(1

InchiKey: VVRPSGPCPLAYQW-UHFFFAOYSA-N

Formula: C12H13ClF8O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 392.67

Physical Properties

Property code	Value	Unit	Source
gf	-1874.17	kJ/mol	Joback Method
hf	-2273.29	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	50.48	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.272		Crippen Method
mcvol	215.350	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	1249.00		NIST Webbook
tb	622.35	K	Joback Method
tc	787.32	K	Joback Method
tf	376.41	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.81	J/mol×K	622.35	Joback Method
cpg	607.84	J/mol×K	649.85	Joback Method
cpg	619.04	J/mol×K	677.34	Joback Method
cpg	629.48	J/mol×K	704.84	Joback Method
cpg	639.19	J/mol×K	732.33	Joback Method
cpg	648.23	J/mol×K	759.83	Joback Method
cpg	656.65	J/mol×K	787.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370669&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume