Diethylmalonic acid, monochloride, 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C11H12ClF7O3/c1-3-8(4-2,6(12)20)7(21)22-5-9(13,14)10(15,16)11(17,18)19/h

InchiKey: QATJCKBVCHBRPL-UHFFFAOYSA-N

Formula: C11H12ClF7O3

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

Mol. weight [g/mol]: 360.65

Physical Properties

Property code	Value	Unit	Source
gf	-1685.34	kJ/mol	Joback Method
hf	-2051.26	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	49.46	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.934		Crippen Method
mcvol	199.490	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
tb	600.64	K	Joback Method
tc	769.28	K	Joback Method
tf	379.55	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.52	J/mol×K	600.64	Joback Method
cpg	549.35	J/mol×K	628.75	Joback Method
cpg	560.35	J/mol×K	656.85	Joback Method
cpg	570.57	J/mol×K	684.96	Joback Method
cpg	580.06	J/mol×K	713.07	Joback Method
cpg	588.87	J/mol×K	741.17	Joback Method
cpg	597.05	J/mol×K	769.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368445&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume