Diethylmalonic acid, monochloride, 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C15H16ClF3O3/c1-3-14(4-2,12(16)20)13(21)22-9-10-5-7-11(8-6-10)15(17,18)1

InchiKey: MKMLKQSWQCRBMT-UHFFFAOYSA-N

Formula: C15H16ClF3O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 336.73

Physical Properties

Property code	Value	Unit	Source
gf	-775.32	kJ/mol	Joback Method
hf	-1106.82	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	67.17	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.320		Crippen Method
mcvol	225.010	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1748.00		NIST Webbook
tb	733.20	K	Joback Method
tc	937.43	K	Joback Method
tf	456.37	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.59	J/mol×K	733.20	Joback Method
cpg	634.52	J/mol×K	767.24	Joback Method
cpg	646.49	J/mol×K	801.28	Joback Method
cpg	657.57	J/mol×K	835.32	Joback Method
cpg	667.82	J/mol×K	869.36	Joback Method
cpg	677.30	J/mol×K	903.39	Joback Method
cpg	686.08	J/mol×K	937.43	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=U368408&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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