Diethylmalonic acid, 2-chloro-6-fluorophenyl propyl ester

Inchi: InChI=1S/C16H20ClFO4/c1-4-10-21-14(19)16(5-2,6-3)15(20)22-13-11(17)8-7-9-12(13)18

InchiKey: LNVSNGDAMZJNMM-UHFFFAOYSA-N

Formula: C16H20ClFO4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 330.78

Physical Properties

Property code	Value	Unit	Source
gf	-494.75	kJ/mol	Joback Method
hf	-870.18	kJ/mol	Joback Method
hfus	35.90	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.144		Crippen Method
mcvol	241.430	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	788.17	K	Joback Method
tc	995.84	K	Joback Method
tf	498.79	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.62	J/mol×K	788.17	Joback Method
cpg	697.23	J/mol×K	822.78	Joback Method
cpg	709.85	J/mol×K	857.39	Joback Method
cpg	721.51	J/mol×K	892.01	Joback Method
cpg	732.23	J/mol×K	926.62	Joback Method
cpg	742.06	J/mol×K	961.23	Joback Method
cpg	751.01	J/mol×K	995.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369672&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

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