

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

Inchi:	InChI=1S/C21H30ClFO4/c1-4-7-8-9-10-11-15-26-19(24)21(5-2,6-3)20(25)27-18-16(22)1
InchiKey:	HEYQYKHJTOFFDW-UHFFFAOYSA-N
Formula:	C21H30ClFO4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	400.91

Physical Properties

Property code	Value	Unit	Source
gf	-452.65	kJ/mol	Joback Method
hf	-973.38	kJ/mol	Joback Method
hfus	48.85	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.095		Crippen Method
mcvol	311.880	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	902.57	K	Joback Method
tc	1110.69	K	Joback Method
tf	555.14	K	Joback Method
vc	1.208	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.22	J/mol×K	902.57	Joback Method
cpg	986.05	J/mol×K	937.26	Joback Method
cpg	999.73	J/mol×K	971.94	Joback Method
cpg	1012.30	J/mol×K	1006.63	Joback Method
cpg	1023.81	J/mol×K	1041.32	Joback Method
cpg	1034.30	J/mol×K	1076.00	Joback Method
cpg	1043.81	J/mol×K	1110.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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