Dimethylmalonic acid, 2-chloro-6-fluorophenyl heptadecyl ester

Inchi: InChI=1S/C28H44ClFO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-33-26(31)28(2,3

InchiKey: XLJMBAGVLMAMHN-UHFFFAOYSA-N

Formula: C28H44ClFO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 499.10

Physical Properties

Property code	Value	Unit	Source
gf	-393.71	kJ/mol	Joback Method
hf	-1117.86	kJ/mol	Joback Method
hfus	66.98	kJ/mol	Joback Method
hvap	102.11	kJ/mol	Joback Method
log10ws	-9.79		Crippen Method
logp	8.825		Crippen Method
mcvol	410.510	ml/mol	McGowan Method
pc	782.00	kPa	Joback Method
rinpol	3191.00		NIST Webbook
rinpol	3191.00		NIST Webbook
tb	1062.73	K	Joback Method
tc	1308.40	K	Joback Method
tf	634.03	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1400.66	J/mol×K	1062.73	Joback Method
cpg	1417.68	J/mol×K	1103.67	Joback Method
cpg	1433.03	J/mol×K	1144.62	Joback Method
cpg	1446.83	J/mol×K	1185.56	Joback Method
cpg	1459.17	J/mol×K	1226.51	Joback Method
cpg	1470.16	J/mol×K	1267.45	Joback Method
cpg	1479.92	J/mol×K	1308.40	Joback Method

Sources

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=U361967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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