Diethylmalonic acid, 2-fluorophenyl tetradecyl ester

Inchi: InChI=1S/C27H43FO4/c1-4-7-8-9-10-11-12-13-14-15-16-19-22-31-25(29)27(5-2,6-3)26(3

InchiKey: GZIUPCVMMPIJRK-UHFFFAOYSA-N

Formula: C27H43FO4

SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F

Mol. weight [g/mol]: 450.63

Physical Properties

Property code	Value	Unit	Source
gf	-380.57	kJ/mol	Joback Method
hf	-1070.01	kJ/mol	Joback Method
hfus	60.58	kJ/mol	Joback Method
hvap	94.83	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.782		Crippen Method
mcvol	384.180	ml/mol	McGowan Method
pc	850.98	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	997.44	K	Joback Method
tc	1222.69	K	Joback Method
tf	580.32	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.03	J/mol×K	997.44	Joback Method
cpg	1330.81	J/mol×K	1034.98	Joback Method
cpg	1347.10	J/mol×K	1072.52	Joback Method
cpg	1361.98	J/mol×K	1110.06	Joback Method
cpg	1375.53	J/mol×K	1147.61	Joback Method
cpg	1387.84	J/mol×K	1185.15	Joback Method
cpg	1398.99	J/mol×K	1222.69	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=U370138&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