Diethylmalonic acid, 2-fluorophenyl hexyl ester

Inchi: InChI=1S/C19H27FO4/c1-4-7-8-11-14-23-17(21)19(5-2,6-3)18(22)24-16-13-10-9-12-15(1

InchiKey: KBYRKTJGIDRLAC-UHFFFAOYSA-N

Formula: C19H27FO4

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

Mol. weight [g/mol]: 338.41

Physical Properties

Property code	Value	Unit	Source
gf	-447.93	kJ/mol	Joback Method
hf	-904.89	kJ/mol	Joback Method
hfus	39.86	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.661		Crippen Method
mcvol	271.460	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	2073.00		NIST Webbook
tb	814.40	K	Joback Method
tc	1014.68	K	Joback Method
tf	490.16	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.83	J/mol×K	814.40	Joback Method
cpg	843.44	J/mol×K	847.78	Joback Method
cpg	857.98	J/mol×K	881.16	Joback Method
cpg	871.48	J/mol×K	914.54	Joback Method
cpg	883.98	J/mol×K	947.92	Joback Method
cpg	895.51	J/mol×K	981.30	Joback Method
cpg	906.12	J/mol×K	1014.68	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=U370130&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