Diethylmalonic acid, 2-fluorophenyl heptyl ester

Inchi: InChI=1S/C20H29FO4/c1-4-7-8-9-12-15-24-18(22)20(5-2,6-3)19(23)25-17-14-11-10-13-1

InchiKey: MUCSPVQZPCGBHZ-UHFFFAOYSA-N

Formula: C20H29FO4

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

Mol. weight [g/mol]: 352.44

Physical Properties

Property code	Value	Unit	Source
gf	-439.51	kJ/mol	Joback Method
hf	-925.53	kJ/mol	Joback Method
hfus	42.45	kJ/mol	Joback Method
hvap	79.25	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.051		Crippen Method
mcvol	285.550	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	2167.00		NIST Webbook
tb	837.28	K	Joback Method
tc	1037.82	K	Joback Method
tf	501.43	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.13	J/mol×K	837.28	Joback Method
cpg	901.96	J/mol×K	870.70	Joback Method
cpg	916.69	J/mol×K	904.13	Joback Method
cpg	930.35	J/mol×K	937.55	Joback Method
cpg	942.98	J/mol×K	970.97	Joback Method
cpg	954.64	J/mol×K	1004.40	Joback Method
cpg	965.34	J/mol×K	1037.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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