Diethylmalonic acid, pentyl 3,4-difluorobenzyl ester

Inchi: InChI=1S/C19H26F2O4/c1-4-7-8-11-24-17(22)19(5-2,6-3)18(23)25-13-14-9-10-15(20)16

InchiKey: QUEALYZFQNRQHR-UHFFFAOYSA-N

Formula: C19H26F2O4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1

Mol. weight [g/mol]: 356.40

Physical Properties

Property code	Value	Unit	Source
gf	-652.37	kJ/mol	Joback Method
hf	-1112.47	kJ/mol	Joback Method
hfus	42.55	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.548		Crippen Method
mcvol	273.230	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	818.65	K	Joback Method
tc	1015.16	K	Joback Method
tf	503.27	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.57	J/mol×K	818.65	Joback Method
cpg	849.65	J/mol×K	851.40	Joback Method
cpg	863.69	J/mol×K	884.15	Joback Method
cpg	876.75	J/mol×K	916.91	Joback Method
cpg	888.83	J/mol×K	949.66	Joback Method
cpg	899.98	J/mol×K	982.41	Joback Method
cpg	910.23	J/mol×K	1015.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U369325&Units=SI

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