Diethylmalonic acid, 3,4-difluorobenzyl decyl ester

Inchi: InChI=1S/C24H36F2O4/c1-4-7-8-9-10-11-12-13-16-29-22(27)24(5-2,6-3)23(28)30-18-19

InchiKey: DBOKVGLVQBSDOR-UHFFFAOYSA-N

Formula: C24H36F2O4

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

Mol. weight [g/mol]: 426.54

Physical Properties

Property code	Value	Unit	Source
gf	-610.27	kJ/mol	Joback Method
hf	-1215.67	kJ/mol	Joback Method
hfus	55.50	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.498		Crippen Method
mcvol	343.680	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook
tb	933.05	K	Joback Method
tc	1142.39	K	Joback Method
tf	559.62	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.01	J/mol×K	933.05	Joback Method
cpg	1149.52	J/mol×K	967.94	Joback Method
cpg	1164.74	J/mol×K	1002.83	Joback Method
cpg	1178.73	J/mol×K	1037.72	Joback Method
cpg	1191.54	J/mol×K	1072.61	Joback Method
cpg	1203.23	J/mol×K	1107.50	Joback Method
cpg	1213.84	J/mol×K	1142.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369330&Units=SI
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

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