Diethylmalonic acid, 3,4-difluorobenzyl nonyl ester

Inchi: InChI=1S/C23H34F2O4/c1-4-7-8-9-10-11-12-15-28-21(26)23(5-2,6-3)22(27)29-17-18-13

InchiKey: TZIGXBHGIFZUJI-UHFFFAOYSA-N

Formula: C23H34F2O4

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

Mol. weight [g/mol]: 412.51

Physical Properties

Property code	Value	Unit	Source
gf	-618.69	kJ/mol	Joback Method
hf	-1195.03	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	85.77	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.108		Crippen Method
mcvol	329.590	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	910.17	K	Joback Method
tc	1115.25	K	Joback Method
tf	548.35	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.00	J/mol×K	910.17	Joback Method
cpg	1088.19	J/mol×K	944.35	Joback Method
cpg	1103.16	J/mol×K	978.53	Joback Method
cpg	1116.96	J/mol×K	1012.71	Joback Method
cpg	1129.63	J/mol×K	1046.89	Joback Method
cpg	1141.23	J/mol×K	1081.07	Joback Method
cpg	1151.79	J/mol×K	1115.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369329&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