Diethylmalonic acid, 3,4-difluorobenzyl octyl ester

Inchi: InChI=1S/C22H32F2O4/c1-4-7-8-9-10-11-14-27-20(25)22(5-2,6-3)21(26)28-16-17-12-13

InchiKey: WGCZELMASVUQOV-UHFFFAOYSA-N

Formula: C22H32F2O4

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

Mol. weight [g/mol]: 398.48

Physical Properties

Property code	Value	Unit	Source
gf	-627.11	kJ/mol	Joback Method
hf	-1174.39	kJ/mol	Joback Method
hfus	50.32	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.718		Crippen Method
mcvol	315.500	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	887.29	K	Joback Method
tc	1089.02	K	Joback Method
tf	537.08	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.59	J/mol×K	887.29	Joback Method
cpg	1027.48	J/mol×K	920.91	Joback Method
cpg	1042.22	J/mol×K	954.53	Joback Method
cpg	1055.83	J/mol×K	988.15	Joback Method
cpg	1068.37	J/mol×K	1021.77	Joback Method
cpg	1079.87	J/mol×K	1055.39	Joback Method
cpg	1090.37	J/mol×K	1089.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369328&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

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