Diethylmalonic acid, di(3,4-difluorobenzyl) ester

Inchi: InChI=1S/C21H20F4O4/c1-3-21(4-2,19(26)28-11-13-5-7-15(22)17(24)9-13)20(27)29-12-
InchiKey: NZOARJUISVSUFV-UHFFFAOYSA-N
Formula: C21H20F4O4
SMILES: CCC(CC)(C(=O)OCc1ccc(F)c(F)c1)C(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 412.37

Physical Properties

Property code	Value	Unit	Source
gf	-932.00	kJ/mol	Joback Method
hf	-1332.38	kJ/mol	Joback Method
hfus	47.15	kJ/mol	Joback Method
hvap	83.29	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	4.836		Crippen Method
mcvol	281.190	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	899.59	K	Joback Method
tc	1110.72	K	Joback Method
tf	578.45	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.59	J/mol×K	899.59	Joback Method
cpg	878.08	J/mol×K	934.78	Joback Method
cpg	889.46	J/mol×K	969.97	Joback Method
cpg	899.76	J/mol×K	1005.15	Joback Method
cpg	909.02	J/mol×K	1040.34	Joback Method
cpg	917.29	J/mol×K	1075.53	Joback Method
cpg	924.61	J/mol×K	1110.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369339&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