Diethylmalonic acid, 3,4-difluorobenzyl ethyl ester

Inchi: InChI=1S/C16H20F2O4/c1-4-16(5-2,14(19)21-6-3)15(20)22-10-11-7-8-12(17)13(18)9-11

InchiKey: HIBNRAXLMZAGIG-UHFFFAOYSA-N

Formula: C16H20F2O4

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

Mol. weight [g/mol]: 314.32

Physical Properties

Property code	Value	Unit	Source
gf	-677.63	kJ/mol	Joback Method
hf	-1050.55	kJ/mol	Joback Method
hfus	34.78	kJ/mol	Joback Method
hvap	70.19	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.377		Crippen Method
mcvol	230.960	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	750.01	K	Joback Method
tc	947.40	K	Joback Method
tf	469.46	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.21	J/mol×K	750.01	Joback Method
cpg	679.40	J/mol×K	782.91	Joback Method
cpg	692.66	J/mol×K	815.81	Joback Method
cpg	705.02	J/mol×K	848.70	Joback Method
cpg	716.49	J/mol×K	881.60	Joback Method
cpg	727.10	J/mol×K	914.50	Joback Method
cpg	736.87	J/mol×K	947.40	Joback Method

Sources

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=U369322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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