Diethylmalonic acid, 3,4-difluorobenzyl isobutyl ester

Inchi: InChI=1S/C18H24F2O4/c1-5-18(6-2,16(21)23-10-12(3)4)17(22)24-11-13-7-8-14(19)15(2
InchiKey: ZICCWDANXNQPTP-UHFFFAOYSA-N
Formula: C18H24F2O4
SMILES: CCC(CC)(C(=O)OCc1ccc(F)c(F)c1)C(=O)OCC(C)C
Mol. weight [g/mol]: 342.38

Physical Properties

Property code	Value	Unit	Source
gf	-663.23	kJ/mol	Joback Method
hf	-1097.11	kJ/mol	Joback Method
hfus	36.44	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.014		Crippen Method
mcvol	259.140	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	1922.00		NIST Webbook
rinpol	1922.00		NIST Webbook
tb	795.33	K	Joback Method
tc	993.67	K	Joback Method
tf	477.00	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.72	J/mol×K	795.33	Joback Method
cpg	792.68	J/mol×K	828.39	Joback Method
cpg	806.62	J/mol×K	861.44	Joback Method
cpg	819.56	J/mol×K	894.50	Joback Method
cpg	831.54	J/mol×K	927.56	Joback Method
cpg	842.58	J/mol×K	960.61	Joback Method
cpg	852.71	J/mol×K	993.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369324&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