Diethylmalonic acid, di(2-fluoro-3-trifluoromethylphenyl) ester

Inchi: InChI=1S/C21H16F8O4/c1-3-19(4-2,17(30)32-13-9-5-7-11(15(13)22)20(24,25)26)18(31)
InchiKey: AIDICFCJTLQJQN-UHFFFAOYSA-N
Formula: C21H16F8O4
SMILES: CCC(CC)(C(=O)Oc1cccc(C(F)(F)F)c1F)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 484.34

Physical Properties

Property code	Value	Unit	Source
gf	-1705.56	kJ/mol	Joback Method
hf	-2134.32	kJ/mol	Joback Method
hfus	44.64	kJ/mol	Joback Method
hvap	77.43	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.320		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2048.00		NIST Webbook
tb	890.21	K	Joback Method
tc	1095.19	K	Joback Method
tf	585.65	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.44	J/mol×K	890.21	Joback Method
cpg	907.75	J/mol×K	924.37	Joback Method
cpg	918.11	J/mol×K	958.54	Joback Method
cpg	927.61	J/mol×K	992.70	Joback Method
cpg	936.31	J/mol×K	1026.86	Joback Method
cpg	944.31	J/mol×K	1061.03	Joback Method
cpg	951.66	J/mol×K	1095.19	Joback Method

Sources

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=U370725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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