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

Inchi: InChI=1S/C19H12F8O4/c1-17(2,15(28)30-11-7-3-5-9(13(11)20)18(22,23)24)16(29)31-12

InchiKey: IIWWKZUQVUTOAD-UHFFFAOYSA-N

Formula: C19H12F8O4

SMILES: CC(C)(C(=O)Oc1cccc(C(F)(F)F)c1F)C(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 456.28

Physical Properties

Property code	Value	Unit	Source
gf	-1722.40	kJ/mol	Joback Method
hf	-2093.04	kJ/mol	Joback Method
hfus	39.46	kJ/mol	Joback Method
hvap	72.98	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.540		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	844.45	K	Joback Method
tc	1046.87	K	Joback Method
tf	563.11	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.31	J/mol×K	844.45	Joback Method
cpg	794.98	J/mol×K	878.19	Joback Method
cpg	804.72	J/mol×K	911.92	Joback Method
cpg	813.62	J/mol×K	945.66	Joback Method
cpg	821.74	J/mol×K	979.39	Joback Method
cpg	829.15	J/mol×K	1013.13	Joback Method
cpg	835.92	J/mol×K	1046.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U362011&Units=SI

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