

Diethylmalonic acid, isobutyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi:	InChI=1S/C18H22F4O4/c1-5-17(6-2,15(23)25-10-11(3)4)16(24)26-13-9-7-8-12(14(13)19
InchiKey:	FONRTWNEKXNCDV-UHFFFAOYSA-N
Formula:	C18H22F4O4
SMILES:	CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1050.01	kJ/mol	Joback Method
hf	-1498.08	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.756		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	790.64	K	Joback Method
tc	984.78	K	Joback Method
tf	480.60	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.51	J/molxK	790.64	Joback Method
cpg	808.72	J/molxK	823.00	Joback Method
cpg	821.94	J/molxK	855.35	Joback Method
cpg	834.22	J/molxK	887.71	Joback Method
cpg	845.60	J/molxK	920.07	Joback Method
cpg	856.13	J/molxK	952.42	Joback Method
cpg	865.85	J/molxK	984.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U370709&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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