Diethylmalonic acid, hexyl 2,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C20H27F3O4/c1-4-7-8-9-10-26-18(24)20(5-2,6-3)19(25)27-13-14-11-16(22)17

InchiKey: GRPOXDHMNCOPEH-UHFFFAOYSA-N

Formula: C20H27F3O4

SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cc(F)c(F)cc1F

Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-848.39	kJ/mol	Joback Method
hf	-1340.69	kJ/mol	Joback Method
hfus	47.83	kJ/mol	Joback Method
hvap	78.94	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.077		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1208.99	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	845.78	K	Joback Method
tc	1040.99	K	Joback Method
tf	527.65	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.45	J/mol×K	845.78	Joback Method
cpg	914.37	J/mol×K	878.31	Joback Method
cpg	928.26	J/mol×K	910.85	Joback Method
cpg	941.14	J/mol×K	943.38	Joback Method
cpg	953.03	J/mol×K	975.92	Joback Method
cpg	963.97	J/mol×K	1008.45	Joback Method
cpg	973.99	J/mol×K	1040.99	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=U369259&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

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