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

Inchi: InChI=1S/C23H32F4O4/c1-4-7-8-9-10-11-12-16-30-20(28)22(5-2,6-3)21(29)31-18-15-13

InchiKey: JWILIEFMYHJUQV-UHFFFAOYSA-N

Formula: C23H32F4O4

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

Mol. weight [g/mol]: 448.49

Physical Properties

Property code	Value	Unit	Source
gf	-1005.47	kJ/mol	Joback Method
hf	-1596.00	kJ/mol	Joback Method
hfus	51.65	kJ/mol	Joback Method
hvap	82.84	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	6.850		Crippen Method
mcvol	333.130	ml/mol	McGowan Method
pc	992.00	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	905.48	K	Joback Method
tc	1108.92	K	Joback Method
tf	551.95	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.61	J/mol×K	905.48	Joback Method
cpg	1102.31	J/mol×K	939.39	Joback Method
cpg	1116.86	J/mol×K	973.29	Joback Method
cpg	1130.35	J/mol×K	1007.20	Joback Method
cpg	1142.82	J/mol×K	1041.11	Joback Method
cpg	1154.36	J/mol×K	1075.02	Joback Method
cpg	1165.02	J/mol×K	1108.92	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=U370714&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

Latest version available from:
https://www.chemeo.com/cid/122-627-0/Diethylmalonic-acid-2-fluoro-3-trifluoromethylphenyl-nonyl-ester.pdf
Generated by Cheméo on 2024-05-01 13:57:14.4853751 +0000 UTC m=+16861083.405952412.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.