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

Inchi: InChI=1S/C21H28F4O4/c1-4-7-8-9-10-14-28-18(26)20(5-2,6-3)19(27)29-16-13-11-12-15

InchiKey: KCBYWAKNFUGMQJ-UHFFFAOYSA-N

Formula: C21H28F4O4

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

Mol. weight [g/mol]: 420.44

Physical Properties

Property code	Value	Unit	Source
gf	-1022.31	kJ/mol	Joback Method
hf	-1554.72	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	78.39	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.070		Crippen Method
mcvol	304.950	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2090.00		NIST Webbook
tb	859.72	K	Joback Method
tc	1056.32	K	Joback Method
tf	529.41	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.28	J/mol×K	859.72	Joback Method
cpg	982.27	J/mol×K	892.49	Joback Method
cpg	996.22	J/mol×K	925.25	Joback Method
cpg	1009.17	J/mol×K	958.02	Joback Method
cpg	1021.17	J/mol×K	990.79	Joback Method
cpg	1032.29	J/mol×K	1023.56	Joback Method
cpg	1042.58	J/mol×K	1056.32	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=U370712&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