Glutaric acid, 2-fluoro-6-(trifluoromethyl)benzyl nonyl ester

Inchi: InChI=1S/C22H30F4O4/c1-2-3-4-5-6-7-8-15-29-20(27)13-10-14-21(28)30-16-17-18(22(2

InchiKey: YWALXXTWCNRKET-UHFFFAOYSA-N

Formula: C22H30F4O4

SMILES: CCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 434.46

Physical Properties

Property code	Value	Unit	Source
gf	-1016.73	kJ/mol	Joback Method
hf	-1566.61	kJ/mol	Joback Method
hfus	56.48	kJ/mol	Joback Method
hvap	81.91	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.352		Crippen Method
mcvol	319.040	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2750.00		NIST Webbook
tb	885.83	K	Joback Method
tc	1084.74	K	Joback Method
tf	538.26	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.97	J/mol×K	885.83	Joback Method
cpg	1041.43	J/mol×K	918.98	Joback Method
cpg	1055.75	J/mol×K	952.13	Joback Method
cpg	1068.98	J/mol×K	985.29	Joback Method
cpg	1081.16	J/mol×K	1018.44	Joback Method
cpg	1092.33	J/mol×K	1051.59	Joback Method
cpg	1102.53	J/mol×K	1084.74	Joback Method

Sources

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=U377505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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