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

Inchi: InChI=1S/C18H22F4O4/c1-2-3-4-11-25-16(23)9-6-10-17(24)26-12-13-14(18(20,21)22)7-

InchiKey: FLTYBWGNLBQLHD-UHFFFAOYSA-N

Formula: C18H22F4O4

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

Mol. weight [g/mol]: 378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1050.41	kJ/mol	Joback Method
hf	-1484.05	kJ/mol	Joback Method
hfus	46.12	kJ/mol	Joback Method
hvap	73.01	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.791		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	2316.00		NIST Webbook
tb	794.31	K	Joback Method
tc	981.98	K	Joback Method
tf	493.18	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.30	J/mol×K	794.31	Joback Method
cpg	806.29	J/mol×K	825.59	Joback Method
cpg	819.36	J/mol×K	856.87	Joback Method
cpg	831.53	J/mol×K	888.15	Joback Method
cpg	842.83	J/mol×K	919.42	Joback Method
cpg	853.30	J/mol×K	950.70	Joback Method
cpg	862.95	J/mol×K	981.98	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=U377500&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