Glutaric acid, hept-2-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C19H24F4O4/c1-3-4-5-8-13(2)26-16(24)11-7-12-17(25)27-15-10-6-9-14(18(15

InchiKey: OQBGTCBEIDTXEQ-UHFFFAOYSA-N

Formula: C19H24F4O4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 392.39

Physical Properties

Property code	Value	Unit	Source
gf	-1044.43	kJ/mol	Joback Method
hf	-1509.97	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	74.85	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.432		Crippen Method
mcvol	276.770	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinpol	2081.00		NIST Webbook
rinpol	2081.00		NIST Webbook
tb	816.75	K	Joback Method
tc	1007.32	K	Joback Method
tf	489.45	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.05	J/mol×K	816.75	Joback Method
cpg	864.49	J/mol×K	848.51	Joback Method
cpg	877.94	J/mol×K	880.27	Joback Method
cpg	890.43	J/mol×K	912.03	Joback Method
cpg	901.99	J/mol×K	943.80	Joback Method
cpg	912.66	J/mol×K	975.56	Joback Method
cpg	922.46	J/mol×K	1007.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393620&Units=SI
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

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