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

Inchi: InChI=1S/C18H22F4O4/c1-4-13(11(2)3)25-15(23)9-6-10-16(24)26-14-8-5-7-12(17(14)19

InchiKey: PLRCRKDTWWJUPS-UHFFFAOYSA-N

Formula: C18H22F4O4

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

Mol. weight [g/mol]: 378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1055.29	kJ/mol	Joback Method
hf	-1494.61	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	72.23	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.898		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	793.43	K	Joback Method
tc	984.31	K	Joback Method
tf	463.18	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.40	J/mol×K	793.43	Joback Method
cpg	807.63	J/mol×K	825.24	Joback Method
cpg	820.89	J/mol×K	857.06	Joback Method
cpg	833.20	J/mol×K	888.87	Joback Method
cpg	844.60	J/mol×K	920.69	Joback Method
cpg	855.12	J/mol×K	952.50	Joback Method
cpg	864.77	J/mol×K	984.31	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=U393616&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