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

Inchi: InChI=1S/C17H20F4O4/c1-10(2)11(3)24-14(22)8-5-9-15(23)25-13-7-4-6-12(16(13)18)17

InchiKey: QPUACUPGKMVSNB-UHFFFAOYSA-N

Formula: C17H20F4O4

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

Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1063.71	kJ/mol	Joback Method
hf	-1473.97	kJ/mol	Joback Method
hfus	36.48	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.508		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	770.55	K	Joback Method
tc	961.03	K	Joback Method
tf	451.91	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.11	J/mol×K	770.55	Joback Method
cpg	751.02	J/mol×K	802.30	Joback Method
cpg	764.00	J/mol×K	834.04	Joback Method
cpg	776.07	J/mol×K	865.79	Joback Method
cpg	787.26	J/mol×K	897.53	Joback Method
cpg	797.58	J/mol×K	929.28	Joback Method
cpg	807.08	J/mol×K	961.03	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=U393615&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