Glutaric acid, 3-methylbut-2-en-1-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C17H18F4O4/c1-11(2)9-10-24-14(22)7-4-8-15(23)25-13-6-3-5-12(16(13)18)17

InchiKey: INXMIJHHWQNFBG-UHFFFAOYSA-N

Formula: C17H18F4O4

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

Mol. weight [g/mol]: 362.32

Physical Properties

Property code	Value	Unit	Source
gf	-987.16	kJ/mol	Joback Method
hf	-1355.98	kJ/mol	Joback Method
hfus	42.42	kJ/mol	Joback Method
hvap	70.82	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.430		Crippen Method
mcvol	244.290	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	775.47	K	Joback Method
tc	968.18	K	Joback Method
tf	462.87	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.57	J/mol×K	775.47	Joback Method
cpg	723.73	J/mol×K	807.59	Joback Method
cpg	736.02	J/mol×K	839.71	Joback Method
cpg	747.49	J/mol×K	871.83	Joback Method
cpg	758.16	J/mol×K	903.94	Joback Method
cpg	768.08	J/mol×K	936.06	Joback Method
cpg	777.27	J/mol×K	968.18	Joback Method

Sources

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=U393617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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