Glutaric acid, 2-fluoro-6-(trifluoromethyl)benzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H26F4O4/c1-4-7-17(13(2)3)28-19(26)11-6-10-18(25)27-12-14-15(20(22,23
InchiKey: RVIIZLPWNGQSPN-UHFFFAOYSA-N
Formula: C20H26F4O4
SMILES: CCCC(OC(=O)CCCC(=O)OCc1c(F)cccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 406.41

Physical Properties

Property code	Value	Unit	Source
gf	-1038.45	kJ/mol	Joback Method
hf	-1535.89	kJ/mol	Joback Method
hfus	44.25	kJ/mol	Joback Method
hvap	76.69	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.426		Crippen Method
mcvol	290.860	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	839.19	K	Joback Method
tc	1032.88	K	Joback Method
tf	485.72	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.63	J/mol×K	839.19	Joback Method
cpg	923.46	J/mol×K	871.47	Joback Method
cpg	937.25	J/mol×K	903.75	Joback Method
cpg	950.01	J/mol×K	936.03	Joback Method
cpg	961.78	J/mol×K	968.32	Joback Method
cpg	972.60	J/mol×K	1000.60	Joback Method
cpg	982.50	J/mol×K	1032.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377501&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

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