Glutaric acid, cyclohexylmethyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C19H22F4O4/c20-18-14(19(21,22)23)8-4-9-15(18)27-17(25)11-5-10-16(24)26-

InchiKey: VLGZZWCFQQWZED-UHFFFAOYSA-N

Formula: C19H22F4O4

SMILES: O=C(CCCC(=O)Oc1cccc(C(F)(F)F)c1F)OCC1CCCCC1

Mol. weight [g/mol]: 390.37

Physical Properties

Property code	Value	Unit	Source
gf	-1017.54	kJ/mol	Joback Method
hf	-1450.37	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.044		Crippen Method
mcvol	265.910	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
tb	836.74	K	Joback Method
tc	1041.71	K	Joback Method
tf	511.83	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.97	J/mol×K	836.74	Joback Method
cpg	858.97	J/mol×K	870.90	Joback Method
cpg	872.73	J/mol×K	905.06	Joback Method
cpg	885.30	J/mol×K	939.23	Joback Method
cpg	896.71	J/mol×K	973.39	Joback Method
cpg	906.99	J/mol×K	1007.55	Joback Method
cpg	916.21	J/mol×K	1041.71	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=U393622&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