Glutaric acid, di(2,3,6-trifluorobenzyl) ester

Inchi: InChI=1S/C19H14F6O4/c20-12-4-6-14(22)18(24)10(12)8-28-16(26)2-1-3-17(27)29-9-11-
InchiKey: BWFGBOHFFPMLNT-UHFFFAOYSA-N
Formula: C19H14F6O4
SMILES: O=C(CCCC(=O)OCc1c(F)ccc(F)c1F)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 420.30

Physical Properties

Property code	Value	Unit	Source
gf	-1360.56	kJ/mol	Joback Method
hf	-1697.51	kJ/mol	Joback Method
hfus	54.77	kJ/mol	Joback Method
hvap	79.82	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	4.478		Crippen Method
mcvol	256.550	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
tb	865.56	K	Joback Method
tc	1065.13	K	Joback Method
tf	579.71	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.53	J/mol×K	865.56	Joback Method
cpg	773.73	J/mol×K	898.82	Joback Method
cpg	783.94	J/mol×K	932.08	Joback Method
cpg	793.16	J/mol×K	965.35	Joback Method
cpg	801.40	J/mol×K	998.61	Joback Method
cpg	808.66	J/mol×K	1031.87	Joback Method
cpg	814.95	J/mol×K	1065.13	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=U376911&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