Glutaric acid, 2-methylhex-3-yl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C19H25F3O4/c1-4-6-16(12(2)3)26-18(24)8-5-7-17(23)25-11-13-14(20)9-10-15

InchiKey: POCZQSPJMYEMQF-UHFFFAOYSA-N

Formula: C19H25F3O4

SMILES: CCCC(OC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F)C(C)C

Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-864.53	kJ/mol	Joback Method
hf	-1321.86	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.685		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	825.25	K	Joback Method
tc	1017.82	K	Joback Method
tf	483.96	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.06	J/mol×K	825.25	Joback Method
cpg	855.83	J/mol×K	857.35	Joback Method
cpg	869.58	J/mol×K	889.44	Joback Method
cpg	882.31	J/mol×K	921.54	Joback Method
cpg	894.04	J/mol×K	953.63	Joback Method
cpg	904.78	J/mol×K	985.73	Joback Method
cpg	914.53	J/mol×K	1017.82	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=U376898&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