Glutaric acid, 3,4-difluorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H26F2O4/c1-4-6-17(13(2)3)25-19(23)8-5-7-18(22)24-12-14-9-10-15(20)16

InchiKey: CZNDNEAIMQVIDR-UHFFFAOYSA-N

Formula: C19H26F2O4

SMILES: CCCC(OC(=O)CCCC(=O)OCc1ccc(F)c(F)c1)C(C)C

Mol. weight [g/mol]: 356.40

Physical Properties

Property code	Value	Unit	Source
gf	-660.09	kJ/mol	Joback Method
hf	-1114.28	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.546		Crippen Method
mcvol	273.230	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	821.00	K	Joback Method
tc	1016.29	K	Joback Method
tf	470.85	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.34	J/mol×K	821.00	Joback Method
cpg	849.57	J/mol×K	853.55	Joback Method
cpg	863.74	J/mol×K	886.10	Joback Method
cpg	876.86	J/mol×K	918.65	Joback Method
cpg	888.96	J/mol×K	951.20	Joback Method
cpg	900.04	J/mol×K	983.74	Joback Method
cpg	910.13	J/mol×K	1016.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377637&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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