Glutaric acid, 1-(2,6-difluorophenyl)ethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H28F2O4/c1-5-8-17(13(2)3)26-19(24)12-7-11-18(23)25-14(4)20-15(21)9-6

InchiKey: BPOJGTKSXBCGIL-UHFFFAOYSA-N

Formula: C20H28F2O4

SMILES: CCCC(OC(=O)CCCC(=O)OC(C)c1c(F)cccc1F)C(C)C

Mol. weight [g/mol]: 370.43

Physical Properties

Property code	Value	Unit	Source
gf	-654.11	kJ/mol	Joback Method
hf	-1140.20	kJ/mol	Joback Method
hfus	41.98	kJ/mol	Joback Method
hvap	79.23	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.107		Crippen Method
mcvol	287.320	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	843.44	K	Joback Method
tc	1041.41	K	Joback Method
tf	467.12	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.35	J/mol×K	843.44	Joback Method
cpg	908.93	J/mol×K	876.44	Joback Method
cpg	923.38	J/mol×K	909.43	Joback Method
cpg	936.70	J/mol×K	942.43	Joback Method
cpg	948.93	J/mol×K	975.42	Joback Method
cpg	960.08	J/mol×K	1008.42	Joback Method
cpg	970.16	J/mol×K	1041.41	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=U377252&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