Glutaric acid, 2-(4-fluorophenyl)ethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H29FO4/c1-4-6-18(15(2)3)25-20(23)8-5-7-19(22)24-14-13-16-9-11-17(21)1

InchiKey: YHWCQRIKARVONB-UHFFFAOYSA-N

Formula: C20H29FO4

SMILES: CCCC(OC(=O)CCCC(=O)OCCc1ccc(F)cc1)C(C)C

Mol. weight [g/mol]: 352.44

Physical Properties

Property code	Value	Unit	Source
gf	-447.23	kJ/mol	Joback Method
hf	-927.34	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	79.77	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.450		Crippen Method
mcvol	285.550	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2350.00		NIST Webbook
tb	839.63	K	Joback Method
tc	1038.94	K	Joback Method
tf	469.01	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.12	J/mol×K	839.63	Joback Method
cpg	902.08	J/mol×K	872.85	Joback Method
cpg	916.89	J/mol×K	906.07	Joback Method
cpg	930.57	J/mol×K	939.29	Joback Method
cpg	943.16	J/mol×K	972.51	Joback Method
cpg	954.68	J/mol×K	1005.72	Joback Method
cpg	965.14	J/mol×K	1038.94	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=U377116&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

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