Glutaric acid, 2-methylpent-3-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H25FO5/c1-5-14(12(2)3)23-17(20)7-6-8-18(21)24-15-10-9-13(19)11-16(15

InchiKey: MZWYIPGPWSSONU-UHFFFAOYSA-N

Formula: C18H25FO5

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc(F)cc1OC)C(C)C

Mol. weight [g/mol]: 340.39

Physical Properties

Property code	Value	Unit	Source
gf	-578.70	kJ/mol	Joback Method
hf	-1029.75	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	78.39	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.888		Crippen Method
mcvol	263.240	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	821.27	K	Joback Method
tc	1021.35	K	Joback Method
tf	481.22	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.76	J/mol×K	821.27	Joback Method
cpg	812.75	J/mol×K	854.62	Joback Method
cpg	826.63	J/mol×K	887.96	Joback Method
cpg	839.38	J/mol×K	921.31	Joback Method
cpg	851.01	J/mol×K	954.65	Joback Method
cpg	861.53	J/mol×K	988.00	Joback Method
cpg	870.93	J/mol×K	1021.35	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=U393441&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