Glutaric acid, 2-ethylhexyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C20H29FO5/c1-4-6-8-15(5-2)14-25-19(22)9-7-10-20(23)26-17-12-11-16(21)13

InchiKey: XRTIBUNULDAMRM-UHFFFAOYSA-N

Formula: C20H29FO5

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 368.44

Physical Properties

Property code	Value	Unit	Source
gf	-559.42	kJ/mol	Joback Method
hf	-1065.75	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	83.23	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.670		Crippen Method
mcvol	291.420	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
tb	867.47	K	Joback Method
tc	1068.00	K	Joback Method
tf	518.76	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.18	J/mol×K	867.47	Joback Method
cpg	929.47	J/mol×K	900.89	Joback Method
cpg	943.54	J/mol×K	934.31	Joback Method
cpg	956.41	J/mol×K	967.74	Joback Method
cpg	968.07	J/mol×K	1001.16	Joback Method
cpg	978.54	J/mol×K	1034.58	Joback Method
cpg	987.82	J/mol×K	1068.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393446&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

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