Glutaric acid, hept-2-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C19H27FO5/c1-4-5-6-8-14(2)24-18(21)9-7-10-19(22)25-16-12-11-15(20)13-17

InchiKey: KENXHSFDRJROBJ-UHFFFAOYSA-N

Formula: C19H27FO5

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

Mol. weight [g/mol]: 354.41

Physical Properties

Property code	Value	Unit	Source
gf	-567.84	kJ/mol	Joback Method
hf	-1045.11	kJ/mol	Joback Method
hfus	44.55	kJ/mol	Joback Method
hvap	81.00	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.422		Crippen Method
mcvol	277.330	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2306.00		NIST Webbook
rinpol	2306.00		NIST Webbook
tb	844.59	K	Joback Method
tc	1043.57	K	Joback Method
tf	507.49	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.32	J/mol×K	844.59	Joback Method
cpg	870.40	J/mol×K	877.75	Joback Method
cpg	884.33	J/mol×K	910.92	Joback Method
cpg	897.12	J/mol×K	944.08	Joback Method
cpg	908.76	J/mol×K	977.25	Joback Method
cpg	919.27	J/mol×K	1010.41	Joback Method
cpg	928.65	J/mol×K	1043.57	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=U393444&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