Glutaric acid, 2-(cyclohexyl)ethyl 2-fluorophenyl ester

Inchi: InChI=1S/C19H25FO4/c20-16-9-4-5-10-17(16)24-19(22)12-6-11-18(21)23-14-13-15-7-2-

InchiKey: HNEKSNRVXOLBNC-UHFFFAOYSA-N

Formula: C19H25FO4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCCC1CCCCC1

Mol. weight [g/mol]: 336.40

Physical Properties

Property code	Value	Unit	Source
gf	-426.32	kJ/mol	Joback Method
hf	-841.82	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	78.75	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.415		Crippen Method
mcvol	260.600	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2404.00		NIST Webbook
rinpol	2404.00		NIST Webbook
tb	837.18	K	Joback Method
tc	1051.53	K	Joback Method
tf	495.12	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.41	J/mol×K	837.18	Joback Method
cpg	837.82	J/mol×K	872.90	Joback Method
cpg	852.84	J/mol×K	908.63	Joback Method
cpg	866.51	J/mol×K	944.35	Joback Method
cpg	878.86	J/mol×K	980.08	Joback Method
cpg	889.90	J/mol×K	1015.80	Joback Method
cpg	899.67	J/mol×K	1051.53	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=U405419&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