Glutaric acid, 2-chloro-6-fluorophenyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H20ClFO5/c25-20-11-5-12-21(26)24(20)31-23(28)14-6-13-22(27)29-16-17
InchiKey: AOBACTVYBIUNRT-UHFFFAOYSA-N
Formula: C24H20ClFO5
SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 442.86

Physical Properties

Property code	Value	Unit	Source
gf	-320.04	kJ/mol	Joback Method
hf	-697.18	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	102.12	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	6.090		Crippen Method
mcvol	312.500	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
tb	1055.20	K	Joback Method
tc	1300.75	K	Joback Method
tf	674.12	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.88	J/mol×K	1055.20	Joback Method
cpg	964.44	J/mol×K	1096.12	Joback Method
cpg	971.37	J/mol×K	1137.05	Joback Method
cpg	976.73	J/mol×K	1177.97	Joback Method
cpg	980.55	J/mol×K	1218.90	Joback Method
cpg	982.88	J/mol×K	1259.82	Joback Method
cpg	983.77	J/mol×K	1300.75	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392131&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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