Glutaric acid, 2-fluorophenyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H21FO5/c25-21-12-4-5-13-22(21)30-24(27)15-7-14-23(26)28-17-18-8-6-11

InchiKey: WLPJJGZTMUPSKB-UHFFFAOYSA-N

Formula: C24H21FO5

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 408.42

Physical Properties

Property code	Value	Unit	Source
gf	-298.48	kJ/mol	Joback Method
hf	-669.97	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	97.08	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.437		Crippen Method
mcvol	300.260	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	3178.00		NIST Webbook
rinpol	3178.00		NIST Webbook
tb	1012.79	K	Joback Method
tc	1252.72	K	Joback Method
tf	631.68	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.12	J/mol×K	1012.79	Joback Method
cpg	950.48	J/mol×K	1052.78	Joback Method
cpg	959.25	J/mol×K	1092.77	Joback Method
cpg	966.49	J/mol×K	1132.76	Joback Method
cpg	972.24	J/mol×K	1172.75	Joback Method
cpg	976.56	J/mol×K	1212.73	Joback Method
cpg	979.47	J/mol×K	1252.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392128&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