Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H20F8O5/c24-20(25)22(28,29)23(30,31)21(26,27)14-35-19(33)11-5-10-18

InchiKey: HUMXYTVTGXOEMU-UHFFFAOYSA-N

Formula: C23H20F8O5

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 528.39

Physical Properties

Property code	Value	Unit	Source
gf	-1767.27	kJ/mol	Joback Method
hf	-2278.69	kJ/mol	Joback Method
hfus	48.66	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.407		Crippen Method
mcvol	322.320	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	943.01	K	Joback Method
tc	1155.05	K	Joback Method
tf	577.86	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.53	J/mol×K	943.01	Joback Method
cpg	1054.24	J/mol×K	978.35	Joback Method
cpg	1064.88	J/mol×K	1013.69	Joback Method
cpg	1074.54	J/mol×K	1049.03	Joback Method
cpg	1083.33	J/mol×K	1084.37	Joback Method
cpg	1091.35	J/mol×K	1119.71	Joback Method
cpg	1098.68	J/mol×K	1155.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392121&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