Glutaric acid, 3-chlorophenyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H21ClO5/c25-19-8-5-12-22(16-19)30-24(27)14-6-13-23(26)28-17-18-7-4-11-21(15-18)29-20-9-2-1-3-10-20/h1-5,7-8,10-12,15-16H,6,9,13-14,17H2

InchiKey: GEYKCJMNEIURQX-UHFFFAOYSA-N

Formula: C24H21ClO5

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 424.87

Physical Properties

Property code	Value	Unit	Source
gf	-115.60	kJ/mol	Joback Method
hf	-489.60	kJ/mol	Joback Method
hfus	50.22	kJ/mol	Joback Method
hvap	102.28	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.951		Crippen Method
mcvol	310.730	ml/mol	McGowan Method
pc	1573.45	kPa	Joback Method
rinpol	3363.00		NIST Webbook
rinpol	3363.00		NIST Webbook
tb	1050.95	K	Joback Method
tc	1300.10	K	Joback Method
tf	661.01	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.11	J/mol×K	1050.95	Joback Method
cpg	960.19	J/mol×K	1092.48	Joback Method
cpg	967.64	J/mol×K	1134.00	Joback Method
cpg	973.51	J/mol×K	1175.53	Joback Method
cpg	977.86	J/mol×K	1217.05	Joback Method
cpg	980.74	J/mol×K	1258.58	Joback Method
cpg	982.21	J/mol×K	1300.10	Joback Method
dvisc	0.0001599	Pa×s	661.01	Joback Method

dvisc	0.0000982	Pa×s	726.00	Joback Method
dvisc	0.0000654	Pa×s	790.99	Joback Method
dvisc	0.0000463	Pa×s	855.98	Joback Method
dvisc	0.0000344	Pa×s	920.97	Joback Method
dvisc	0.0000266	Pa×s	985.96	Joback Method
dvisc	0.0000212	Pa×s	1050.95	Joback Method

Sources

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=U392132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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