Glutaric acid, 2-methylpent-3-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H30O5/c1-4-22(18(2)3)29-24(26)15-9-14-23(25)27-17-19-10-8-13-21(16-1

InchiKey: SESUWORTJNCCAT-UHFFFAOYSA-N

Formula: C24H30O5

SMILES: CCC(OC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1)C(C)C

Mol. weight [g/mol]: 398.49

Physical Properties

Property code	Value	Unit	Source
gf	-211.33	kJ/mol	Joback Method
hf	-709.48	kJ/mol	Joback Method
hfus	45.32	kJ/mol	Joback Method
hvap	94.18	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.670		Crippen Method
mcvol	322.250	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2900.00		NIST Webbook
rinpol	2900.00		NIST Webbook
tb	980.98	K	Joback Method
tc	1208.20	K	Joback Method
tf	562.15	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.03	J/mol×K	980.98	Joback Method
cpg	1097.20	J/mol×K	1170.33	Joback Method
cpg	1089.80	J/mol×K	1132.46	Joback Method
cpg	1080.92	J/mol×K	1094.59	Joback Method
cpg	1070.53	J/mol×K	1056.72	Joback Method
cpg	1058.58	J/mol×K	1018.85	Joback Method
cpg	1103.16	J/mol×K	1208.20	Joback Method
dvisc	0.0000195	Pa×s	980.98	Joback Method

dvisc	0.0000257	Pa×s	911.17	Joback Method
dvisc	0.0000354	Pa×s	841.37	Joback Method
dvisc	0.0000517	Pa×s	771.57	Joback Method
dvisc	0.0000814	Pa×s	701.76	Joback Method
dvisc	0.0001417	Pa×s	631.95	Joback Method
dvisc	0.0002829	Pa×s	562.15	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=U392124&Units=SI

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