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

Inchi: InChI=1S/C25H32O5/c1-3-4-6-11-20(2)29-25(27)17-10-16-24(26)28-19-21-12-9-15-23(1
InchiKey: HIJHXBZQBZGPQT-UHFFFAOYSA-N
Formula: C25H32O5
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 412.52

Physical Properties

Property code	Value	Unit	Source
gf	-200.47	kJ/mol	Joback Method
hf	-724.84	kJ/mol	Joback Method
hfus	51.44	kJ/mol	Joback Method
hvap	96.79	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.204		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	1004.30	K	Joback Method
tc	1232.41	K	Joback Method
tf	588.42	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.72	J/mol×K	1004.30	Joback Method
cpg	1118.21	J/mol×K	1042.32	Joback Method
cpg	1130.08	J/mol×K	1080.34	Joback Method
cpg	1140.37	J/mol×K	1118.36	Joback Method
cpg	1149.13	J/mol×K	1156.38	Joback Method
cpg	1156.41	J/mol×K	1194.39	Joback Method
cpg	1162.23	J/mol×K	1232.41	Joback Method
dvisc	0.0002284	Pa×s	588.42	Joback Method

dvisc	0.0001204	Pa×s	657.73	Joback Method
dvisc	0.0000717	Pa×s	727.05	Joback Method
dvisc	0.0000467	Pa×s	796.36	Joback Method
dvisc	0.0000326	Pa×s	865.67	Joback Method
dvisc	0.0000240	Pa×s	934.99	Joback Method
dvisc	0.0000184	Pa×s	1004.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392127&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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