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

Inchi: InChI=1S/C28H38O5/c1-3-4-5-6-7-9-14-23(2)32-28(30)20-13-19-27(29)31-22-24-15-12-1

InchiKey: PAHBXWFGGASUFM-UHFFFAOYSA-N

Formula: C28H38O5

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

Mol. weight [g/mol]: 454.60

Physical Properties

Property code	Value	Unit	Source
gf	-175.21	kJ/mol	Joback Method
hf	-786.76	kJ/mol	Joback Method
hfus	59.21	kJ/mol	Joback Method
hvap	103.47	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.375		Crippen Method
mcvol	378.610	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
rinpol	3302.00		NIST Webbook
rinpol	3302.00		NIST Webbook
tb	1072.94	K	Joback Method
tc	1313.86	K	Joback Method
tf	622.23	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.17	J/mol×K	1072.94	Joback Method
cpg	1300.58	J/mol×K	1113.09	Joback Method
cpg	1312.12	J/mol×K	1153.25	Joback Method
cpg	1321.87	J/mol×K	1193.40	Joback Method
cpg	1329.90	J/mol×K	1233.55	Joback Method
cpg	1336.25	J/mol×K	1273.70	Joback Method
cpg	1341.01	J/mol×K	1313.86	Joback Method
dvisc	0.0001568	Pa×s	622.23	Joback Method

dvisc	0.0000804	Pa×s	697.35	Joback Method
dvisc	0.0000469	Pa×s	772.47	Joback Method
dvisc	0.0000301	Pa×s	847.58	Joback Method
dvisc	0.0000208	Pa×s	922.70	Joback Method
dvisc	0.0000152	Pa×s	997.82	Joback Method
dvisc	0.0000116	Pa×s	1072.94	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=U392133&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