Adipic acid, decyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C29H40O5/c1-2-3-4-5-6-7-8-14-22-32-28(30)20-12-13-21-29(31)33-24-25-16-1
InchiKey: UDRNHBZMGMAOAA-UHFFFAOYSA-N
Formula: C29H40O5
SMILES: CCCCCCCCCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 468.62

Physical Properties

Property code	Value	Unit	Source
gf	-164.35	kJ/mol	Joback Method
hf	-802.12	kJ/mol	Joback Method
hfus	65.32	kJ/mol	Joback Method
hvap	106.08	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.766		Crippen Method
mcvol	392.700	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	3487.00		NIST Webbook
rinpol	3487.00		NIST Webbook
tb	1096.26	K	Joback Method
tc	1344.67	K	Joback Method
tf	648.50	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.42	J/mol×K	1096.26	Joback Method
cpg	1397.26	J/mol×K	1303.27	Joback Method
cpg	1391.12	J/mol×K	1261.87	Joback Method
cpg	1383.24	J/mol×K	1220.47	Joback Method
cpg	1373.55	J/mol×K	1179.06	Joback Method
cpg	1361.96	J/mol×K	1137.66	Joback Method
cpg	1401.74	J/mol×K	1344.67	Joback Method
dvisc	0.0000109	Pa×s	1096.26	Joback Method

dvisc	0.0000142	Pa×s	1021.63	Joback Method
dvisc	0.0000192	Pa×s	947.01	Joback Method
dvisc	0.0000273	Pa×s	872.38	Joback Method
dvisc	0.0000415	Pa×s	797.75	Joback Method
dvisc	0.0000689	Pa×s	723.13	Joback Method
dvisc	0.0001285	Pa×s	648.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353820&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