Adipic acid, octyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C27H36O5/c1-2-3-4-5-6-12-20-30-26(28)18-10-11-19-27(29)31-22-23-14-13-1
InchiKey: PAMLPZXIVVYYPV-UHFFFAOYSA-N
Formula: C27H36O5
SMILES: CCCCCCCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 440.57

Physical Properties

Property code	Value	Unit	Source
gf	-181.19	kJ/mol	Joback Method
hf	-760.84	kJ/mol	Joback Method
hfus	60.14	kJ/mol	Joback Method
hvap	101.63	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.986		Crippen Method
mcvol	364.520	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1050.50	K	Joback Method
tc	1286.11	K	Joback Method
tf	625.96	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.77	J/mol×K	1050.50	Joback Method
cpg	1276.39	J/mol×K	1246.84	Joback Method
cpg	1269.54	J/mol×K	1207.57	Joback Method
cpg	1261.11	J/mol×K	1168.31	Joback Method
cpg	1251.04	J/mol×K	1129.04	Joback Method
cpg	1239.28	J/mol×K	1089.77	Joback Method
cpg	1281.71	J/mol×K	1286.11	Joback Method
dvisc	0.0000149	Pa×s	1050.50	Joback Method

dvisc	0.0000193	Pa×s	979.74	Joback Method
dvisc	0.0000259	Pa×s	908.99	Joback Method
dvisc	0.0000366	Pa×s	838.23	Joback Method
dvisc	0.0000552	Pa×s	767.47	Joback Method
dvisc	0.0000904	Pa×s	696.72	Joback Method
dvisc	0.0001654	Pa×s	625.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353818&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