Adipic acid, pentyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H30O5/c1-2-3-9-17-27-23(25)15-7-8-16-24(26)28-19-20-11-10-14-22(18-2
InchiKey: BLLGSZKJGOAEOB-UHFFFAOYSA-N
Formula: C24H30O5
SMILES: CCCCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 398.49

Physical Properties

Property code	Value	Unit	Source
gf	-206.45	kJ/mol	Joback Method
hf	-698.92	kJ/mol	Joback Method
hfus	52.37	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.816		Crippen Method
mcvol	322.250	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook
tb	981.86	K	Joback Method
tc	1206.57	K	Joback Method
tf	592.15	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.22	J/mol×K	981.86	Joback Method
cpg	1057.73	J/mol×K	1019.31	Joback Method
cpg	1069.72	J/mol×K	1056.76	Joback Method
cpg	1080.21	J/mol×K	1094.22	Joback Method
cpg	1089.24	J/mol×K	1131.67	Joback Method
cpg	1096.85	J/mol×K	1169.12	Joback Method
cpg	1103.08	J/mol×K	1206.57	Joback Method
dvisc	0.0002370	Pa×s	592.15	Joback Method

dvisc	0.0001334	Pa×s	657.10	Joback Method
dvisc	0.0000832	Pa×s	722.05	Joback Method
dvisc	0.0000561	Pa×s	787.00	Joback Method
dvisc	0.0000402	Pa×s	851.96	Joback Method
dvisc	0.0000302	Pa×s	916.91	Joback Method
dvisc	0.0000236	Pa×s	981.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353814&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