

Adipic acid, 3-phenoxybenzyl undecyl ester

Inchi: InChI=1S/C30H42O5/c1-2-3-4-5-6-7-8-9-15-23-33-29(31)21-13-14-22-30(32)34-25-26-17
InchiKey: CHBDBNIQKDSFFF-UHFFFAOYSA-N
Formula: C30H42O5
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 482.65

Physical Properties

Property code	Value	Unit	Source
gf	-155.93	kJ/mol	Joback Method
hf	-822.76	kJ/mol	Joback Method
hfus	67.91	kJ/mol	Joback Method
hvap	108.31	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.157		Crippen Method
mcvol	406.790	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	3606.00		NIST Webbook
tb	1119.14	K	Joback Method
tc	1375.85	K	Joback Method
tf	659.77	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.11	J/molxK	1119.14	Joback Method
cpg	1457.90	J/molxK	1333.06	Joback Method
cpg	1452.18	J/molxK	1290.28	Joback Method
cpg	1444.63	J/molxK	1247.49	Joback Method
cpg	1435.16	J/molxK	1204.71	Joback Method
cpg	1423.68	J/molxK	1161.92	Joback Method
cpg	1461.88	J/molxK	1375.85	Joback Method
dvisc	0.0000093	Paxs	1119.14	Joback Method
dvisc	0.0000121	Paxs	1042.58	Joback Method

dvisc	0.0000164	Paxs	966.02	Joback Method
dvisc	0.0000235	Paxs	889.45	Joback Method
dvisc	0.0000359	Paxs	812.89	Joback Method
dvisc	0.0000600	Paxs	736.33	Joback Method
dvisc	0.0001128	Paxs	659.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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