

Adipic acid, heptyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C26H34O5/c1-2-3-4-5-11-19-29-25(27)17-9-10-18-26(28)30-21-22-13-12-16-2
InchiKey:	XZOC DHSNCCUEEV-UHFFFAOYSA-N
Formula:	C26H34O5
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	426.55

Physical Properties

Property code	Value	Unit	Source
gf	-189.61	kJ/mol	Joback Method
hf	-740.20	kJ/mol	Joback Method
hfus	57.55	kJ/mol	Joback Method
hvap	99.41	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.596		Crippen Method
mcvol	350.430	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpola	3188.00		NIST Webbook
tb	1027.62	K	Joback Method
tc	1258.56	K	Joback Method
tf	614.69	K	Joback Method
vc	1.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.89	J/molxK	1027.62	Joback Method
cpg	1178.39	J/molxK	1066.11	Joback Method
cpg	1190.24	J/molxK	1104.60	Joback Method
cpg	1200.46	J/molxK	1143.09	Joback Method
cpg	1209.12	J/molxK	1181.58	Joback Method
cpg	1216.26	J/molxK	1220.07	Joback Method
cpg	1221.93	J/molxK	1258.56	Joback Method
dvisc	0.0001870	Paxs	614.69	Joback Method
dvisc	0.0001032	Paxs	683.51	Joback Method

dvisc	0.0000634	Paxs	752.33	Joback Method
dvisc	0.0000423	Paxs	821.15	Joback Method
dvisc	0.0000301	Paxs	889.98	Joback Method
dvisc	0.0000224	Paxs	958.80	Joback Method
dvisc	0.0000174	Paxs	1027.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353817&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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