

Phthalic acid, pentadecyl 2-propylphenyl ester

Inchi:	InChI=1S/C32H46O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-20-26-35-31(33)28-23-17-18-24
InchiKey:	UFYCTYLAFMBFKP-UHFFFAOYSA-N
Formula:	C32H46O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1CCC
Mol. weight [g/mol]:	494.71

Physical Properties

Property code	Value	Unit	Source
gf	-43.72	kJ/mol	Joback Method
hf	-743.29	kJ/mol	Joback Method
hfus	71.51	kJ/mol	Joback Method
hvap	111.01	kJ/mol	Joback Method
log10ws	-10.88		Crippen Method
logp	9.106		Crippen Method
mcvol	429.100	ml/mol	McGowan Method
pc	786.39	kPa	Joback Method
rinsol	3551.00		NIST Webbook
tb	1147.46	K	Joback Method
tc	1416.05	K	Joback Method
tf	672.60	K	Joback Method
vc	1.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1508.60	J/molxK	1147.46	Joback Method
cpg	1523.83	J/molxK	1192.22	Joback Method
cpg	1536.99	J/molxK	1236.99	Joback Method
cpg	1548.22	J/molxK	1281.75	Joback Method
cpg	1557.64	J/molxK	1326.52	Joback Method
cpg	1565.38	J/molxK	1371.28	Joback Method
cpg	1571.57	J/molxK	1416.05	Joback Method
dvisc	0.0001143	Paxs	672.60	Joback Method
dvisc	0.0000609	Paxs	751.74	Joback Method

dvisc	0.0000366	Paxs	830.89	Joback Method
dvisc	0.0000240	Paxs	910.03	Joback Method
dvisc	0.0000168	Paxs	989.17	Joback Method
dvisc	0.0000125	Paxs	1068.32	Joback Method
dvisc	0.0000096	Paxs	1147.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357030&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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