

Phthalic acid, 2,4-dimethylpent-3-yl undecyl ester

Inchi:	InChI=1S/C26H42O4/c1-6-7-8-9-10-11-12-13-16-19-29-25(27)22-17-14-15-18-23(22)26(
InchiKey:	FIKFQEARQFOQQG-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCOC(=O)c1cccc1C(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-204.34	kJ/mol	Joback Method
hf	-860.35	kJ/mol	Joback Method
hfus	51.75	kJ/mol	Joback Method
hvap	93.56	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.212		Crippen Method
mvol	368.320	ml/mol	McGowan Method
pc	928.37	kPa	Joback Method
rinpol	2798.00		NIST Webbook
tb	977.20	K	Joback Method
tc	1196.38	K	Joback Method
tf	521.04	K	Joback Method
vc	1.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.76	J/molxK	977.20	Joback Method
cpg	1316.33	J/molxK	1159.85	Joback Method
cpg	1304.96	J/molxK	1123.32	Joback Method
cpg	1292.17	J/molxK	1086.79	Joback Method
cpg	1277.90	J/molxK	1050.26	Joback Method
cpg	1262.12	J/molxK	1013.73	Joback Method
cpg	1326.32	J/molxK	1196.38	Joback Method
dvisc	0.0000172	Paxs	977.20	Joback Method
dvisc	0.0000235	Paxs	901.17	Joback Method

dvisc	0.0000339	Paxs	825.15	Joback Method
dvisc	0.0000527	Paxs	749.12	Joback Method
dvisc	0.0000905	Paxs	673.09	Joback Method
dvisc	0.0001785	Paxs	597.07	Joback Method
dvisc	0.0004292	Paxs	521.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356850&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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