

Phthalic acid, pent-4-enyl undecyl ester

Inchi: InChI=1S/C24H36O4/c1-3-5-7-8-9-10-11-12-16-20-28-24(26)22-18-14-13-17-21(22)23(24)25
InchiKey: JZVXADSKOKEQNT-UHFFFAOYSA-N
Formula: C24H36O4
SMILES: C=CCCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-126.02	kJ/mol	Joback Method
hf	-677.80	kJ/mol	Joback Method
hfus	55.86	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.497		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2748.00		NIST Webbook
tb	929.44	K	Joback Method
tc	1138.95	K	Joback Method
tf	541.74	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.34	J/mol×K	929.44	Joback Method
cpg	1106.90	J/mol×K	964.36	Joback Method
cpg	1122.17	J/mol×K	999.28	Joback Method
cpg	1136.18	J/mol×K	1034.19	Joback Method
cpg	1148.97	J/mol×K	1069.11	Joback Method
cpg	1160.59	J/mol×K	1104.03	Joback Method
cpg	1171.08	J/mol×K	1138.95	Joback Method
dvisc	0.0003970	Pa×s	541.74	Joback Method
dvisc	0.0002105	Pa×s	606.36	Joback Method

dvisc	0.0001262	Pa×s	670.97	Joback Method
dvisc	0.0000827	Pa×s	735.59	Joback Method
dvisc	0.0000581	Pa×s	800.21	Joback Method
dvisc	0.0000430	Pa×s	864.82	Joback Method
dvisc	0.0000332	Pa×s	929.44	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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