

Phthalic acid, pent-4-enyl tridecyl ester

Inchi:	InChI=1S/C26H40O4/c1-3-5-7-8-9-10-11-12-13-14-18-22-30-26(28)24-20-16-15-19-23(2
InchiKey:	IJWVSMQETQOBPD-UHFFFAOYSA-N
Formula:	C26H40O4
SMILES:	C=CCCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]:	416.59

Physical Properties

Property code	Value	Unit	Source
gf	-109.18	kJ/mol	Joback Method
hf	-719.08	kJ/mol	Joback Method
hfus	61.04	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.277		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	938.64	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2955.00		NIST Webbook
tb	975.20	K	Joback Method
tc	1194.07	K	Joback Method
tf	564.28	K	Joback Method
vc	1.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.85	J/molxK	975.20	Joback Method
cpg	1285.48	J/molxK	1157.59	Joback Method
cpg	1273.85	J/molxK	1121.12	Joback Method
cpg	1260.92	J/molxK	1084.64	Joback Method
cpg	1246.65	J/molxK	1048.16	Joback Method
cpg	1230.98	J/molxK	1011.68	Joback Method
cpg	1295.89	J/molxK	1194.07	Joback Method
dvisc	0.0000246	Paxs	975.20	Joback Method

dvisc	0.0000321	Paxs	906.71	Joback Method
dvisc	0.0000436	Paxs	838.23	Joback Method
dvisc	0.0000626	Paxs	769.74	Joback Method
dvisc	0.0000966	Paxs	701.25	Joback Method
dvisc	0.0001635	Paxs	632.77	Joback Method
dvisc	0.0003147	Paxs	564.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360472&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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