

Phthalic acid, pent-4-enyl tetradecyl ester

Inchi:	InChI=1S/C27H42O4/c1-3-5-7-8-9-10-11-12-13-14-15-19-23-31-27(29)25-21-17-16-20-2
InchiKey:	SRJGONFEMGGXPQ-UHFFFAOYSA-N
Formula:	C27H42O4
SMILES:	C=CCCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	430.62

Physical Properties

Property code	Value	Unit	Source
gf	-100.76	kJ/mol	Joback Method
hf	-739.72	kJ/mol	Joback Method
hfus	63.63	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.668		Crippen Method
mcvol	378.110	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinsol	3058.00		NIST Webbook
tb	998.08	K	Joback Method
tc	1223.21	K	Joback Method
tf	575.55	K	Joback Method
vc	1.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.31	J/molxK	998.08	Joback Method
cpg	1293.76	J/molxK	1035.60	Joback Method
cpg	1309.66	J/molxK	1073.12	Joback Method
cpg	1324.07	J/molxK	1110.64	Joback Method
cpg	1337.06	J/molxK	1148.16	Joback Method
cpg	1348.69	J/molxK	1185.69	Joback Method
cpg	1359.03	J/molxK	1223.21	Joback Method
dvisc	0.0002789	Paxs	575.55	Joback Method
dvisc	0.0001436	Paxs	645.97	Joback Method

dvisc	0.0000842	Paxs	716.39	Joback Method
dvisc	0.0000543	Paxs	786.82	Joback Method
dvisc	0.0000377	Paxs	857.24	Joback Method
dvisc	0.0000276	Paxs	927.66	Joback Method
dvisc	0.0000212	Paxs	998.08	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=U360473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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