

Phthalic acid, 3-methylbut-3-enyl tetradecyl ester

Inchi:	InChI=1S/C27H42O4/c1-4-5-6-7-8-9-10-11-12-13-14-17-21-30-26(28)24-18-15-16-19-25
InchiKey:	JVYDJNSWBHGNFQ-UHFFFAOYSA-N
Formula:	C27H42O4
SMILES:	C=C(C)CCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	430.62

Physical Properties

Property code	Value	Unit	Source
gf	-109.31	kJ/mol	Joback Method
hf	-749.51	kJ/mol	Joback Method
hfus	62.32	kJ/mol	Joback Method
hvap	96.36	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.668		Crippen Method
mvol	378.110	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	997.96	K	Joback Method
tc	1222.59	K	Joback Method
tf	561.59	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.98	J/molxK	997.96	Joback Method
cpg	1293.43	J/molxK	1035.40	Joback Method
cpg	1309.34	J/molxK	1072.84	Joback Method
cpg	1323.78	J/molxK	1110.27	Joback Method
cpg	1336.82	J/molxK	1147.71	Joback Method
cpg	1348.52	J/molxK	1185.15	Joback Method
cpg	1358.93	J/molxK	1222.59	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=U357112&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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