

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

Inchi:	InChI=1S/C28H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-22-31-27(29)25-19-16-17-20
InchiKey:	YSJSDFYCZAEOBK-UHFFFAOYSA-N
Formula:	C28H44O4
SMILES:	C=C(C)CCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	444.65

Physical Properties

Property code	Value	Unit	Source
gf	-100.89	kJ/mol	Joback Method
hf	-770.15	kJ/mol	Joback Method
hfus	64.91	kJ/mol	Joback Method
hvap	98.58	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.058		Crippen Method
mvol	392.200	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinpol	3143.00		NIST Webbook
rinpol	3143.00		NIST Webbook
tb	1020.84	K	Joback Method
tc	1252.51	K	Joback Method
tf	572.86	K	Joback Method
vc	1.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1338.87	J/molxK	1020.84	Joback Method
cpg	1356.65	J/molxK	1059.45	Joback Method
cpg	1372.80	J/molxK	1098.06	Joback Method
cpg	1387.38	J/molxK	1136.68	Joback Method
cpg	1400.48	J/molxK	1175.29	Joback Method
cpg	1412.16	J/molxK	1213.90	Joback Method
cpg	1422.50	J/molxK	1252.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
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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