

Phthalic acid, 2,4-dimethylpent-3-yl pentadecyl ester

Inchi:	InChI=1S/C30H50O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-20-23-33-29(31)26-21-18-19-
InchiKey:	MUDGAJVXWSJWKM-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	474.72

Physical Properties

Property code	Value	Unit	Source
gf	-170.66	kJ/mol	Joback Method
hf	-942.91	kJ/mol	Joback Method
hfus	62.11	kJ/mol	Joback Method
hvap	102.46	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	8.772		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	744.07	kPa	Joback Method
rinqol	3207.00		NIST Webbook
tb	1068.72	K	Joback Method
tc	1316.96	K	Joback Method
tf	566.12	K	Joback Method
vc	1.637	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.35	J/molxK	1068.72	Joback Method
cpg	1515.66	J/molxK	1110.09	Joback Method
cpg	1531.93	J/molxK	1151.47	Joback Method
cpg	1546.23	J/molxK	1192.84	Joback Method
cpg	1558.67	J/molxK	1234.21	Joback Method
cpg	1569.33	J/molxK	1275.59	Joback Method
cpg	1578.31	J/molxK	1316.96	Joback Method
dvisc	0.0002467	Paxs	566.12	Joback Method
dvisc	0.0001000	Paxs	649.89	Joback Method

dvisc	0.0000498	Paxs	733.65	Joback Method
dvisc	0.0000286	Paxs	817.42	Joback Method
dvisc	0.0000182	Paxs	901.19	Joback Method
dvisc	0.0000125	Paxs	984.95	Joback Method
dvisc	0.0000091	Paxs	1068.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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