

Phthalic acid, propyl 2-tert-butyl-6-methylphenyl ester

Inchi:	InChI=1S/C22H26O4/c1-6-14-25-20(23)16-11-7-8-12-17(16)21(24)26-19-15(2)10-9-13-1
InchiKey:	QVZQTXABIZFE-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	CCCOC(=O)c1ccccc1C(=O)Oc1c(C)cccc1C(C)(C)C
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-134.71	kJ/mol	Joback Method
hf	-557.11	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	88.12	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.079		Crippen Method
mvol	288.200	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	2462.00		NIST Webbook
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tb	920.41	K	Joback Method
tc	1150.27	K	Joback Method
tf	574.84	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.28	J/molxK	920.41	Joback Method
cpg	910.66	J/molxK	958.72	Joback Method
cpg	923.71	J/molxK	997.03	Joback Method
cpg	935.47	J/molxK	1035.34	Joback Method
cpg	946.02	J/molxK	1073.65	Joback Method
cpg	955.41	J/molxK	1111.96	Joback Method
cpg	963.70	J/molxK	1150.27	Joback Method
dvisc	0.0002884	Paxs	574.84	Joback Method

dvisc	0.0001717	Paxs	632.44	Joback Method
dvisc	0.0001115	Paxs	690.03	Joback Method
dvisc	0.0000774	Paxs	747.62	Joback Method
dvisc	0.0000566	Paxs	805.22	Joback Method
dvisc	0.0000431	Paxs	862.82	Joback Method
dvisc	0.0000340	Paxs	920.41	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=U357093&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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