

Phthalic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C24H38O4/c1-17(13-23(3,4)5)15-27-21(25)19-11-9-10-12-20(19)22(26)28-16-
InchiKey: LTKXIKQHSDOYMD-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CC(COC(=O)c1ccccc1C(=O)OCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-213.06	kJ/mol	Joback Method
hf	-831.29	kJ/mol	Joback Method
hfus	35.27	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.145		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	925.42	K	Joback Method
tc	1141.24	K	Joback Method
tf	518.34	K	Joback Method
vc	1.286	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.67	J/molxK	925.42	Joback Method
cpg	1137.92	J/molxK	961.39	Joback Method
cpg	1153.87	J/molxK	997.36	Joback Method
cpg	1168.61	J/molxK	1033.33	Joback Method
cpg	1182.22	J/molxK	1069.30	Joback Method
cpg	1194.78	J/molxK	1105.27	Joback Method
cpg	1206.37	J/molxK	1141.24	Joback Method
dvisc	0.0003972	Paxs	518.34	Joback Method

dvisc	0.0001683	Paxs	586.19	Joback Method
dvisc	0.0000852	Paxs	654.03	Joback Method
dvisc	0.0000490	Paxs	721.88	Joback Method
dvisc	0.0000310	Paxs	789.73	Joback Method
dvisc	0.0000211	Paxs	857.57	Joback Method
dvisc	0.0000152	Paxs	925.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377785&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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