

Phthalic acid, 2,3-dimethylphenyl hexyl ester

Inchi:	InChI=1S/C22H26O4/c1-4-5-6-9-15-25-21(23)18-12-7-8-13-19(18)22(24)26-20-14-10-11
InchiKey:	WTJKEQFITWUUBS-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	CCCCCOC(=O)c1ccccc1C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-137.55	kJ/mol	Joback Method
hf	-548.36	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.260		Crippen Method
mvol	288.200	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2675.00		NIST Webbook
tb	923.64	K	Joback Method
tc	1146.93	K	Joback Method
tf	572.42	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.70	J/molxK	923.64	Joback Method
cpg	909.81	J/molxK	960.86	Joback Method
cpg	922.57	J/molxK	998.07	Joback Method
cpg	934.00	J/molxK	1035.29	Joback Method
cpg	944.15	J/molxK	1072.50	Joback Method
cpg	953.03	J/molxK	1109.72	Joback Method
cpg	960.67	J/molxK	1146.93	Joback Method
dvisc	0.0003310	Paxs	572.42	Joback Method
dvisc	0.0002025	Paxs	630.96	Joback Method

dvisc	0.0001347	Paxs	689.49	Joback Method
dvisc	0.0000955	Paxs	748.03	Joback Method
dvisc	0.0000711	Paxs	806.57	Joback Method
dvisc	0.0000552	Paxs	865.10	Joback Method
dvisc	0.0000442	Paxs	923.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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