

Terephthalic acid, hexyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C22H34O4/c1-6-7-8-9-14-25-20(23)18-10-12-19(13-11-18)21(24)26-16-17(2)1
InchiKey:	NOMNXOSRCGZZDQ-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCC(C)CC(C)(C)C)cc1
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-230.30	kJ/mol	Joback Method
hf	-775.98	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	84.13	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.653		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2662.00		NIST Webbook
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tb	883.33	K	Joback Method
tc	1091.23	K	Joback Method
tf	508.38	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.32	J/molxK	883.33	Joback Method
cpg	1015.05	J/molxK	917.98	Joback Method
cpg	1030.54	J/molxK	952.63	Joback Method
cpg	1044.85	J/molxK	987.28	Joback Method
cpg	1058.01	J/molxK	1021.93	Joback Method
cpg	1070.07	J/molxK	1056.58	Joback Method
cpg	1081.10	J/molxK	1091.23	Joback Method
dvisc	0.0004944	Paxs	508.38	Joback Method

dvisc	0.0002388	Paxs	570.87	Joback Method
dvisc	0.0001332	Paxs	633.36	Joback Method
dvisc	0.0000825	Paxs	695.86	Joback Method
dvisc	0.0000553	Paxs	758.35	Joback Method
dvisc	0.0000394	Paxs	820.84	Joback Method
dvisc	0.0000294	Paxs	883.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416012&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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