

Terephthalic acid, 2-methylpent-3-yl octyl ester

Inchi:	InChI=1S/C22H34O4/c1-5-7-8-9-10-11-16-25-21(23)18-12-14-19(15-13-18)22(24)26-20(
InchiKey:	HIPVPGMYUNTYNU-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCCCCOC(=O)c1ccc(C(=O)OC(CC)C(C)C)cc1
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-235.58	kJ/mol	Joback Method
hf	-772.51	kJ/mol	Joback Method
hfus	44.92	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.795		Crippen Method
mvol	311.960	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	2556.00		NIST Webbook
tb	886.12	K	Joback Method
tc	1091.62	K	Joback Method
tf	490.96	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.25	J/molxK	886.12	Joback Method
cpg	1014.95	J/molxK	920.37	Joback Method
cpg	1030.37	J/molxK	954.62	Joback Method
cpg	1044.54	J/molxK	988.87	Joback Method
cpg	1057.48	J/molxK	1023.12	Joback Method
cpg	1069.24	J/molxK	1057.37	Joback Method
cpg	1079.83	J/molxK	1091.62	Joback Method
dvisc	0.0006178	Paxs	490.96	Joback Method
dvisc	0.0002874	Paxs	556.82	Joback Method

dvisc	0.0001572	Paxs	622.68	Joback Method
dvisc	0.0000965	Paxs	688.54	Joback Method
dvisc	0.0000645	Paxs	754.40	Joback Method
dvisc	0.0000460	Paxs	820.26	Joback Method
dvisc	0.0000345	Paxs	886.12	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=U356199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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