

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

Inchi: InChI=1S/C29H48O4/c1-6-7-8-9-10-11-12-13-14-15-16-21-32-27(30)25-17-19-26(20-18-
InchiKey: ROSOJLYZZVTLRH-UHFFFAOYSA-N
Formula: C29H48O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(C)CC(C)(C)C)cc1
Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-171.36	kJ/mol	Joback Method
hf	-920.46	kJ/mol	Joback Method
hfus	59.15	kJ/mol	Joback Method
hvap	99.71	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	8.383		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	785.95	kPa	Joback Method
rinpol	2628.00		NIST Webbook
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tb	1043.49	K	Joback Method
tc	1280.94	K	Joback Method
tf	587.27	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.20	J/molxK	1043.49	Joback Method
cpg	1509.66	J/molxK	1241.37	Joback Method
cpg	1497.27	J/molxK	1201.79	Joback Method
cpg	1483.54	J/molxK	1162.22	Joback Method
cpg	1468.35	J/molxK	1122.64	Joback Method
cpg	1451.61	J/molxK	1083.07	Joback Method
cpg	1520.81	J/molxK	1280.94	Joback Method
dvisc	0.0000097	Paxs	1043.49	Joback Method

dvisc	0.0000132	Paxs	967.45	Joback Method
dvisc	0.0000188	Paxs	891.42	Joback Method
dvisc	0.0000287	Paxs	815.38	Joback Method
dvisc	0.0000477	Paxs	739.34	Joback Method
dvisc	0.0000892	Paxs	663.31	Joback Method
dvisc	0.0001963	Paxs	587.27	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=U416019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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