

Terephthalic acid, 5-methylhex-2-yl tridecyl ester

Inchi:	InChI=1S/C28H46O4/c1-5-6-7-8-9-10-11-12-13-14-15-22-31-27(29)25-18-20-26(21-19-2
InchiKey:	BLBSKDUWLKMDPV-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)CCC(C)C)cc1
Mol. weight [g/mol]:	446.66

Physical Properties

Property code	Value	Unit	Source
gf	-185.06	kJ/mol	Joback Method
hf	-896.35	kJ/mol	Joback Method
hfus	60.46	kJ/mol	Joback Method
hvap	98.40	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	8.136		Crippen Method
mvol	396.500	ml/mol	McGowan Method
pc	824.79	kPa	Joback Method
rinpol	3566.00		NIST Webbook
rinpol	3566.00		NIST Webbook
tb	1023.40	K	Joback Method
tc	1255.68	K	Joback Method
tf	558.58	K	Joback Method
vc	1.532	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.15	J/molxK	1023.40	Joback Method
cpg	1388.07	J/molxK	1062.11	Joback Method
cpg	1404.21	J/molxK	1100.83	Joback Method
cpg	1418.64	J/molxK	1139.54	Joback Method
cpg	1431.44	J/molxK	1178.25	Joback Method
cpg	1442.65	J/molxK	1216.97	Joback Method
cpg	1452.37	J/molxK	1255.68	Joback Method
dvisc	0.0002898	Paxs	558.58	Joback Method

dvisc	0.0001282	Paxs	636.05	Joback Method
dvisc	0.0000677	Paxs	713.52	Joback Method
dvisc	0.0000405	Paxs	790.99	Joback Method
dvisc	0.0000266	Paxs	868.46	Joback Method
dvisc	0.0000187	Paxs	945.93	Joback Method
dvisc	0.0000138	Paxs	1023.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383006&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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