

Terephthalic acid, 3-methylbut-2-yl hexadecyl ester

Inchi:	InChI=1S/C29H48O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-32-28(30)26-19-21-2
InchiKey:	POCDSYVEOJCBQD-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)C(C)C)cc1
Mol. weight [g/mol]:	460.69

Physical Properties

Property code	Value	Unit	Source
gf	-176.64	kJ/mol	Joback Method
hf	-916.99	kJ/mol	Joback Method
hfus	63.05	kJ/mol	Joback Method
hvap	100.62	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.526		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	781.12	kPa	Joback Method
rinpol	3303.00		NIST Webbook
rinpol	3303.00		NIST Webbook
tb	1046.28	K	Joback Method
tc	1286.84	K	Joback Method
tf	569.85	K	Joback Method
vc	1.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.52	J/molxK	1046.28	Joback Method
cpg	1506.29	J/molxK	1246.75	Joback Method
cpg	1495.24	J/molxK	1206.65	Joback Method
cpg	1482.52	J/molxK	1166.56	Joback Method
cpg	1468.04	J/molxK	1126.47	Joback Method
cpg	1451.74	J/molxK	1086.37	Joback Method
cpg	1515.75	J/molxK	1286.84	Joback Method
dvisc	0.0000118	Paxs	1046.28	Joback Method

dvisc	0.0000160	Paxs	966.88	Joback Method
dvisc	0.0000228	Paxs	887.47	Joback Method
dvisc	0.0000348	Paxs	808.06	Joback Method
dvisc	0.0000584	Paxs	728.66	Joback Method
dvisc	0.0001111	Paxs	649.25	Joback Method
dvisc	0.0002531	Paxs	569.85	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=U356284&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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