Terephthalic acid, hept-3-yl hexadecyl ester

Other names: Terephthalic acid, heptyl-3 hexadecyl ester
Inchi: InChI=1S/C31H52O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-26-34-30(32)27-22-24
InchiKey: JIMDUFHPQPLFIQ-UHFFFAOYSA-N
Formula: C31H52O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(CC)CCCC)cc1
Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-157.36	kJ/mol	Joback Method
hf	-952.99	kJ/mol	Joback Method
hfus	71.75	kJ/mol	Joback Method
hvap	105.46	kJ/mol	Joback Method
log10ws	-10.86		Crippen Method
logp	9.450		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	700.61	kPa	Joback Method
rinpol	3483.00		NIST Webbook
rinpol	3483.00		NIST Webbook
tb	1092.48	K	Joback Method
tc	1356.26	K	Joback Method
tf	607.39	K	Joback Method
vc	1.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1560.96	J/mol×K	1092.48	Joback Method
cpg	1580.15	J/mol×K	1136.44	Joback Method
cpg	1597.09	J/mol×K	1180.41	Joback Method
cpg	1611.87	J/mol×K	1224.37	Joback Method
cpg	1624.62	J/mol×K	1268.34	Joback Method
cpg	1635.46	J/mol×K	1312.30	Joback Method
cpg	1644.50	J/mol×K	1356.26	Joback Method

dvisc	0.0001743	Pa×s	607.39	Joback Method
dvisc	0.0000806	Pa×s	688.24	Joback Method
dvisc	0.0000439	Pa×s	769.09	Joback Method
dvisc	0.0000268	Pa×s	849.93	Joback Method
dvisc	0.0000178	Pa×s	930.78	Joback Method
dvisc	0.0000127	Pa×s	1011.63	Joback Method
dvisc	0.0000095	Pa×s	1092.48	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=U356651&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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