

Isophthalic acid, hept-3-yl hexadecyl ester

Inchi:	InChI=1S/C31H52O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-25-34-30(32)27-22-21
InchiKey:	GGAFKXAWDCXGNF-UHFFFAOYSA-N
Formula:	C31H52O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)CCCC)c1
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	3429.00		NIST Webbook
tb	1092.48	K	Joback Method
tc	1356.26	K	Joback Method
tf	607.39	K	Joback Method
vc	1.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1560.96	J/molxK	1092.48	Joback Method
cpg	1580.15	J/molxK	1136.44	Joback Method
cpg	1597.09	J/molxK	1180.41	Joback Method
cpg	1611.87	J/molxK	1224.37	Joback Method
cpg	1624.62	J/molxK	1268.34	Joback Method
cpg	1635.46	J/molxK	1312.30	Joback Method
cpg	1644.50	J/molxK	1356.26	Joback Method
dvisc	0.0001743	Paxs	607.39	Joback Method
dvisc	0.0000806	Paxs	688.24	Joback Method

dvisc	0.0000439	Paxs	769.09	Joback Method
dvisc	0.0000268	Paxs	849.93	Joback Method
dvisc	0.0000178	Paxs	930.78	Joback Method
dvisc	0.0000127	Paxs	1011.63	Joback Method
dvisc	0.0000095	Paxs	1092.48	Joback Method

Sources

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=U356524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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