

Phthalic acid, hept-4-yl octadecyl ester

Inchi:	InChI=1S/C33H56O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-28-36-32(34)30-
InchiKey:	ZVYDPUXWYCNVRW-UHFFFAOYSA-N
Formula:	C33H56O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OC(CCC)CCC
Mol. weight [g/mol]:	516.80

Physical Properties

Property code	Value	Unit	Source
gf	-140.52	kJ/mol	Joback Method
hf	-994.27	kJ/mol	Joback Method
hfus	76.93	kJ/mol	Joback Method
hvap	109.91	kJ/mol	Joback Method
log10ws	-11.70		Crippen Method
logp	10.230		Crippen Method
mcvol	466.950	ml/mol	McGowan Method
pc	634.48	kPa	Joback Method
rinpol	3525.00		NIST Webbook
tb	1138.24	K	Joback Method
tc	1429.88	K	Joback Method
tf	629.93	K	Joback Method
vc	1.817	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1689.47	J/molxK	1138.24	Joback Method
cpg	1709.60	J/molxK	1186.85	Joback Method
cpg	1727.00	J/molxK	1235.45	Joback Method
cpg	1741.86	J/molxK	1284.06	Joback Method
cpg	1754.36	J/molxK	1332.66	Joback Method
cpg	1764.66	J/molxK	1381.27	Joback Method
cpg	1772.94	J/molxK	1429.88	Joback Method
dvisc	0.0001320	Paxs	629.93	Joback Method
dvisc	0.0000602	Paxs	714.65	Joback Method

dvisc	0.0000324	Paxs	799.37	Joback Method
dvisc	0.0000196	Paxs	884.08	Joback Method
dvisc	0.0000130	Paxs	968.80	Joback Method
dvisc	0.0000092	Paxs	1053.52	Joback Method
dvisc	0.0000068	Paxs	1138.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356799&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

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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