

Phthalic acid, octadecyl pent-4-enyl ester

Inchi: InChI=1S/C31H50O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-23-27-35-31(33)29-2
InchiKey: MWFDHAYJSNSOJR-UHFFFAOYSA-N
Formula: C31H50O4
SMILES: C=CCCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 486.73

Physical Properties

Property code	Value	Unit	Source
gf	-67.08	kJ/mol	Joback Method
hf	-822.28	kJ/mol	Joback Method
hfus	73.99	kJ/mol	Joback Method
hvap	105.18	kJ/mol	Joback Method
log10ws	-10.60		Crippen Method
logp	9.228		Crippen Method
mcvol	434.470	ml/mol	McGowan Method
pc	713.39	kPa	Joback Method
rinpol	3465.00		NIST Webbook
tb	1089.60	K	Joback Method
tc	1352.16	K	Joback Method
tf	620.63	K	Joback Method
vc	1.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1529.81	J/molxK	1089.60	Joback Method
cpg	1605.69	J/molxK	1308.40	Joback Method
cpg	1594.21	J/molxK	1264.64	Joback Method
cpg	1581.00	J/molxK	1220.88	Joback Method
cpg	1565.95	J/molxK	1177.12	Joback Method
cpg	1548.93	J/molxK	1133.36	Joback Method
cpg	1615.58	J/molxK	1352.16	Joback Method
dvisc	0.0000113	Paxs	1089.60	Joback Method
dvisc	0.0000149	Paxs	1011.44	Joback Method

dvisc	0.0000206	Paxs	933.28	Joback Method
dvisc	0.0000301	Paxs	855.12	Joback Method
dvisc	0.0000476	Paxs	776.95	Joback Method
dvisc	0.0000833	Paxs	698.79	Joback Method
dvisc	0.0001676	Paxs	620.63	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=U360477&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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