Phthalic acid, octadecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C34H58O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-26-37-32(35)30-
InchiKey: YCWOUWJQUNXFGN-UHFFFAOYSA-N
Formula: C34H58O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 530.82

Physical Properties

Property code	Value	Unit	Source
gf	-129.26	kJ/mol	Joback Method
hf	-1023.66	kJ/mol	Joback Method
hfus	72.11	kJ/mol	Joback Method
hvap	110.84	kJ/mol	Joback Method
log10ws	-11.52		Crippen Method
logp	10.334		Crippen Method
mcvol	481.040	ml/mol	McGowan Method
pc	610.57	kPa	Joback Method
rinpol	3498.00		NIST Webbook
tb	1157.89	K	Joback Method
tc	1453.05	K	Joback Method
tf	643.62	K	Joback Method
vc	1.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1755.10	J/mol×K	1157.89	Joback Method
cpg	1776.16	J/mol×K	1207.08	Joback Method
cpg	1794.88	J/mol×K	1256.28	Joback Method
cpg	1811.51	J/mol×K	1305.47	Joback Method
cpg	1826.28	J/mol×K	1354.66	Joback Method
cpg	1839.44	J/mol×K	1403.86	Joback Method
cpg	1851.24	J/mol×K	1453.05	Joback Method
dvisc	0.0000952	Pa×s	643.62	Joback Method
dvisc	0.0000418	Pa×s	729.33	Joback Method

dvisc	0.0000218	Pa×s	815.04	Joback Method
dvisc	0.0000129	Pa×s	900.75	Joback Method
dvisc	0.0000083	Pa×s	986.47	Joback Method
dvisc	0.0000058	Pa×s	1072.18	Joback Method
dvisc	0.0000042	Pa×s	1157.89	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=U377784&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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