Benzoic acid, octadecyl ester

Other names: octadecyl benzoate
Inchi: InChI=1S/C25H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-27-25(26)24-21-18
InchiKey: KPWVFNOPNOTYNJ-UHFFFAOYSA-N
Formula: C25H42O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 374.60
CAS: 10578-34-4

Physical Properties

Property code	Value	Unit	Source
gf	38.11	kJ/mol	Joback Method
hf	-567.60	kJ/mol	Joback Method
hfus	57.33	kJ/mol	Joback Method
hvap	82.68	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.105		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	952.01	kPa	Joback Method
rinpol	2843.20		NIST Webbook
rinpol	2860.00		NIST Webbook
tb	874.37	K	Joback Method
tc	1072.27	K	Joback Method
tf	470.09	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.86	J/mol×K	874.37	Joback Method
cpg	1149.45	J/mol×K	907.35	Joback Method
cpg	1167.82	J/mol×K	940.34	Joback Method
cpg	1185.01	J/mol×K	973.32	Joback Method
cpg	1201.09	J/mol×K	1006.30	Joback Method
cpg	1216.10	J/mol×K	1039.29	Joback Method

cpg	1230.10	J/mol×K	1072.27	Joback Method
dvisc	0.0007543	Pa×s	470.09	Joback Method
dvisc	0.0003330	Pa×s	537.47	Joback Method
dvisc	0.0001764	Pa×s	604.85	Joback Method
dvisc	0.0001061	Pa×s	672.23	Joback Method
dvisc	0.0000700	Pa×s	739.61	Joback Method
dvisc	0.0000495	Pa×s	806.99	Joback Method
dvisc	0.0000370	Pa×s	874.37	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=C10578344&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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