

2-Propenoic acid, 2-methyl-, octadecyl ester

Other names:	Methacrylic acid, octadecyl ester Octadecyl methacrylate
Inchi:	InChI=1S/C22H42O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-22(23)21(2)
InchiKey:	HMZGPNHSPWNGEP-UHFFFAOYSA-N
Formula:	C22H42O2
SMILES:	<chem>C=C(C)C(=O)OCCCCCCCCCCCCCCCCCC</chem>
Mol. weight [g/mol]:	338.57
CAS:	32360-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-20.27	kJ/mol	Joback Method
hf	-626.57	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	73.13	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.367		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	954.37	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2377.00		NIST Webbook
ripol	2645.00		NIST Webbook
ripol	2645.00		NIST Webbook
tb	775.61	K	Joback Method
tc	953.12	K	Joback Method
tf	394.14	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.06	J/molxK	775.61	Joback Method

cpg	1024.17	J/mol×K	805.19	Joback Method
cpg	1043.27	J/mol×K	834.78	Joback Method
cpg	1061.41	J/mol×K	864.36	Joback Method
cpg	1078.61	J/mol×K	893.95	Joback Method
cpg	1094.90	J/mol×K	923.53	Joback Method
cpg	1110.33	J/mol×K	953.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32360057&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
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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