

Methacrylic acid, heptadecyl ester

Inchi:	InChI=1S/C21H40O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-21(22)20(2)3/h2
InchiKey:	PAIQEFSJYGYULU-UHFFFAOYSA-N
Formula:	C21H40O2
SMILES:	C=C(C)C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	324.54

Physical Properties

Property code	Value	Unit	Source
gf	-28.69	kJ/mol	Joback Method
hf	-605.93	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.977		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinsol	2278.00		NIST Webbook
tb	752.73	K	Joback Method
tc	927.79	K	Joback Method
tf	382.87	K	Joback Method
vc	1.218	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.96	J/mol×K	752.73	Joback Method
cpg	962.63	J/mol×K	781.91	Joback Method
cpg	981.34	J/mol×K	811.08	Joback Method
cpg	999.14	J/mol×K	840.26	Joback Method
cpg	1016.03	J/mol×K	869.44	Joback Method
cpg	1032.07	J/mol×K	898.61	Joback Method
cpg	1047.27	J/mol×K	927.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340293&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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