2-Propenoic acid, 2-methyl-, hexadecyl ester

Other names: Hexadecyl methacrylate
Methacrylic acid, hexadecyl ester
Inchi: InChI=1S/C20H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-20(21)19(2)3/h2,4-
InchiKey: ZNAOFAIBVOMLPV-UHFFFAOYSA-N
Formula: C20H38O2
SMILES: C=C(C)C(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.51
CAS: 2495-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-37.11	kJ/mol	Joback Method
hf	-585.29	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	68.68	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.587		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2171.00		NIST Webbook
rinpol	2171.00		NIST Webbook
rinpol	2158.00		NIST Webbook
ripol	2446.00		NIST Webbook
tb	729.85	K	Joback Method
tc	903.10	K	Joback Method
tf	371.60	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.78	J/mol×K	729.85	Joback Method
cpg	902.03	J/mol×K	758.73	Joback Method

cpg	920.37	J/mol×K	787.60	Joback Method
cpg	937.83	J/mol×K	816.48	Joback Method
cpg	954.44	J/mol×K	845.35	Joback Method
cpg	970.21	J/mol×K	874.23	Joback Method
cpg	985.18	J/mol×K	903.10	Joback Method
hvapt	73.10	kJ/mol	486.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2495274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume