

E-13-OCTADECEN-1-OL ACETATE

Inchi: InChI=1S/C20H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-20(2)21/h6-7H
InchiKey: PPNRRQMJESAXGJ-VOTSOKGWSA-N
Formula: C20H38O2
SMILES: CCCC/C=C/CCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 310.52

Physical Properties

Property code	Value	Unit	Source
af	0.8804		Cheméo Relay (1.0)
hf	-690.69	kJ/mol	Cheméo Relay (1.0)
hfus	50.54	kJ/mol	Joback Method
hvap	105.61	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	Cheméo Relay (1.0)
log10ws	-6.67		Cheméo Relay (1.0)
logp	6.587		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2200.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
tb	593.74	K	Cheméo Relay (1.0)
tc	773.61	K	Cheméo Relay (1.0)
tf	284.82	K	Cheméo Relay (1.0)
vc	1.124	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.45	J/mol×K	737.45	Joback Method
cpg	904.58	J/mol×K	766.53	Joback Method
cpg	922.81	J/mol×K	795.61	Joback Method
cpg	940.17	J/mol×K	824.69	Joback Method
cpg	956.69	J/mol×K	853.77	Joback Method
cpg	972.40	J/mol×K	882.85	Joback Method

cpg	987.32	J/mol×K	911.93	Joback Method
dvisc	0.0015546	Pa×s	382.24	Joback Method
dvisc	0.0006381	Pa×s	441.44	Joback Method
dvisc	0.0003233	Pa×s	500.64	Joback Method
dvisc	0.0001891	Pa×s	559.85	Joback Method
dvisc	0.0001226	Pa×s	619.05	Joback Method
dvisc	0.0000857	Pa×s	678.25	Joback Method
dvisc	0.0000635	Pa×s	737.45	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U130939&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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