

CYCLOOCTADECANE, ETHYL-

Inchi: InChI=1S/C20H40/c1-2-20-18-16-14-12-10-8-6-4-3-5-7-9-11-13-15-17-19-20/h20H,2-19H
InchiKey: FNBICTKTBOBEOK-UHFFFAOYSA-N
Formula: C20H40
SMILES: CCC1CCCCCCCCCCCCCCCCC1
Mol. weight [g/mol]: 280.54

Physical Properties

Property code	Value	Unit	Source
af	0.2604		Cheméo Relay (1.0)
gf	-3.23	kJ/mol	Joback Method
hf	-470.49	kJ/mol	Cheméo Relay (1.0)
hfus	14.19	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-7.61		Cheméo Relay (1.0)
logp	7.658		Crippen Method
mcvol	281.800	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
tb	658.87	K	Cheméo Relay (1.0)
tc	827.46	K	Cheméo Relay (1.0)
tf	269.80	K	Cheméo Relay (1.0)
vc	0.911	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.41	J/mol×K	727.79	Joback Method
cpg	923.56	J/mol×K	769.23	Joback Method
cpg	954.72	J/mol×K	810.67	Joback Method
cpg	982.83	J/mol×K	852.11	Joback Method
cpg	1007.85	J/mol×K	893.55	Joback Method
cpg	1029.73	J/mol×K	934.99	Joback Method
cpg	1048.40	J/mol×K	976.43	Joback Method
dvisc	0.0912409	Pa×s	280.30	Joback Method

dvisc	0.0023535	Pa×s	354.88	Joback Method
dvisc	0.0002162	Pa×s	429.46	Joback Method
dvisc	0.0000403	Pa×s	504.04	Joback Method
dvisc	0.0000116	Pa×s	578.63	Joback Method
dvisc	0.0000044	Pa×s	653.21	Joback Method
dvisc	0.0000021	Pa×s	727.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U151225&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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