

Crotonic acid, octyl ester, trans-

Inchi:	InChI=1S/C12H22O2/c1-3-5-6-7-8-9-11-14-12(13)10-4-2/h4,10H,3,5-9,11H2,1-2H3/b10-
InchiKey:	HULBECQFWZPEBI-ONNFQVAWSA-N
Formula:	C12H22O2
SMILES:	CC=CC(=O)OCCCCCCCC
Mol. weight [g/mol]:	198.30
CAS:	173605-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-103.54	kJ/mol	Joback Method
hf	-418.59	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
tb	554.41	K	Joback Method
tc	730.90	K	Joback Method
tf	292.08	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.74	J/mol×K	554.41	Joback Method
cpg	461.06	J/mol×K	583.82	Joback Method
cpg	475.72	J/mol×K	613.24	Joback Method
cpg	489.74	J/mol×K	642.65	Joback Method
cpg	503.13	J/mol×K	672.07	Joback Method
cpg	515.92	J/mol×K	701.48	Joback Method
cpg	528.11	J/mol×K	730.90	Joback Method
dvisc	0.0028734	Pa×s	292.08	Joback Method
dvisc	0.0012967	Pa×s	335.80	Joback Method

dvisc	0.0007029	Pa×s	379.52	Joback Method
dvisc	0.0004324	Pa×s	423.25	Joback Method
dvisc	0.0002914	Pa×s	466.97	Joback Method
dvisc	0.0002101	Pa×s	510.69	Joback Method
dvisc	0.0001595	Pa×s	554.41	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C173605135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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

Latest version available from:

<https://www.chemeo.com/cid/12-184-4/Crotonic-acid-octyl-ester-trans.pdf>

Generated by Cheméo on 2025-12-23 06:35:28.291032866 +0000 UTC m=+6219925.821073536.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.