dodec-2-en-4-one

Inchi: InChI=1S/C12H22O/c1-3-5-6-7-8-9-11-12(13)10-4-2/h4,10H,3,5-9,11H2,1-2H3/b10-4+
InchiKey: RBDKOLXWSXOZLC-ONNFQVAWSA-N
Formula: C12H22O
SMILES: CC=CC(=O)CCCCCCCC
Mol. weight [g/mol]: 182.30
CAS: 65570-26-5

Physical Properties

Property code	Value	Unit	Source
gf	1.46	kJ/mol	Joback Method
hf	-286.37	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.882		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
ripol	1905.00		NIST Webbook
tb	531.99	K	Joback Method
tc	709.19	K	Joback Method
tf	269.85	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.56	J/mol×K	531.99	Joback Method
cpg	489.87	J/mol×K	679.66	Joback Method
cpg	476.93	J/mol×K	650.12	Joback Method
cpg	463.35	J/mol×K	620.59	Joback Method
cpg	449.11	J/mol×K	591.06	Joback Method
cpg	434.19	J/mol×K	561.52	Joback Method
cpg	502.21	J/mol×K	709.19	Joback Method
dvisc	0.0001963	Pa×s	531.99	Joback Method

dvisc	0.0002597	Pa×s	488.30	Joback Method
dvisc	0.0003629	Pa×s	444.61	Joback Method
dvisc	0.0005455	Pa×s	400.92	Joback Method
dvisc	0.0009059	Pa×s	357.23	Joback Method
dvisc	0.0017328	Pa×s	313.54	Joback Method
dvisc	0.0040892	Pa×s	269.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65570265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume