

Carbonic acid, heptyl prop-1-en-2-yl ester

Inchi: InChI=1S/C11H20O3/c1-4-5-6-7-8-9-13-11(12)14-10(2)3/h2,4-9H2,1,3H3
InchiKey: VSNDNDUYBQQANI-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: C=C(C)OC(=O)OCCCCCCC
Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-217.89	kJ/mol	Joback Method
hf	-531.75	kJ/mol	Joback Method
hfus	25.63	kJ/mol	Joback Method
hvap	51.06	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.644		Crippen Method
mvol	174.860	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1313.00		NIST Webbook
tb	546.35	K	Joback Method
tc	722.55	K	Joback Method
tf	292.40	K	Joback Method
vc	0.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.38	J/mol×K	546.35	Joback Method
cpg	436.78	J/mol×K	575.72	Joback Method
cpg	450.63	J/mol×K	605.08	Joback Method
cpg	463.92	J/mol×K	634.45	Joback Method
cpg	476.66	J/mol×K	663.82	Joback Method
cpg	488.84	J/mol×K	693.18	Joback Method
cpg	500.48	J/mol×K	722.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382541&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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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