

Propyl 2,4-hexadienecarboxylate

Inchi:	InChI=1S/C9H14O2/c1-3-5-6-7-9(10)11-8-4-2/h3,5-7H,4,8H2,1-2H3/b5-3+,7-6+
InchiKey:	JAVXBQKCKGHZHM-TWTPFVCWSA-N
Formula:	C9H14O2
SMILES:	CC=CC=CC(=O)OCCC
Mol. weight [g/mol]:	154.21
CAS:	88973-62-0

Physical Properties

Property code	Value	Unit	Source
gf	-48.58	kJ/mol	Joback Method
hf	-239.45	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	44.70	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.072		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1366.00		NIST Webbook
tb	489.93	K	Joback Method
tc	679.85	K	Joback Method
tf	253.19	K	Joback Method
vc	0.523	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.90	J/molxK	489.93	Joback Method
cpg	301.42	J/molxK	521.58	Joback Method
cpg	313.33	J/molxK	553.24	Joback Method
cpg	324.65	J/molxK	584.89	Joback Method
cpg	335.41	J/molxK	616.54	Joback Method
cpg	345.63	J/molxK	648.20	Joback Method
cpg	355.33	J/molxK	679.85	Joback Method
dvisc	0.0028409	Paxs	253.19	Joback Method

dvisc	0.0012927	Paxs	292.65	Joback Method
dvisc	0.0007092	Paxs	332.10	Joback Method
dvisc	0.0004420	Paxs	371.56	Joback Method
dvisc	0.0003017	Paxs	411.02	Joback Method
dvisc	0.0002201	Paxs	450.47	Joback Method
dvisc	0.0001690	Paxs	489.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C88973620&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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