

trans-Carvyl formate

Inchi:	InChI=1S/C11H16O2/c1-8(2)10-5-4-9(3)11(6-10)13-7-12/h4,7,10-11H,1,5-6H2,2-3H3/t10
InchiKey:	BPBPWBGJZQBEKD-MNOVXSKEA-N
Formula:	C11H16O2
SMILES:	C=C(C)C1CC=C(C)C(OC=O)C1
Mol. weight [g/mol]:	180.24

Physical Properties

Property code	Value	Unit	Source
gf	-46.42	kJ/mol	Joback Method
hf	-292.24	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	49.69	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.460		Crippen Method
mvol	153.830	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1273.00		NIST Webbook
tb	537.74	K	Joback Method
tc	745.94	K	Joback Method
tf	278.66	K	Joback Method
vc	0.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.30	J/mol×K	537.74	Joback Method
cpg	384.12	J/mol×K	572.44	Joback Method
cpg	400.09	J/mol×K	607.14	Joback Method
cpg	415.22	J/mol×K	641.84	Joback Method
cpg	429.52	J/mol×K	676.54	Joback Method
cpg	443.00	J/mol×K	711.24	Joback Method
cpg	455.66	J/mol×K	745.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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