

Diethyl tetrahydropyran-4,4-dicarboxylate

Inchi:	InChI=1S/C11H18O5/c1-3-15-9(12)11(10(13)16-4-2)5-7-14-8-6-11/h3-8H2,1-2H3
InchiKey:	ILUMJWCFQOFDMA-UHFFFAOYSA-N
Formula:	C11H18O5
SMILES:	CCOC(=O)C1(C(=O)OCC)CCOCC1
Mol. weight [g/mol]:	230.26
CAS:	5382-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-493.26	kJ/mol	Joback Method
hf	-822.41	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	62.18	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.909		Crippen Method
mcvol	175.740	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
tb	650.40	K	Joback Method
tc	863.92	K	Joback Method
tf	415.90	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.20	J/molxK	650.40	Joback Method
cpg	500.02	J/molxK	685.99	Joback Method
cpg	515.04	J/molxK	721.57	Joback Method
cpg	529.33	J/molxK	757.16	Joback Method
cpg	542.99	J/molxK	792.75	Joback Method
cpg	556.08	J/molxK	828.33	Joback Method
cpg	568.68	J/molxK	863.92	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=C5382774&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
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

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