3,6-Dimethyl-4,5,6,7-tetrahydrobenzofuran-2(3H)-o

Inchi: InChI=1S/C10H14O2/c1-6-3-4-8-7(2)10(11)12-9(8)5-6/h6-7H,3-5H2,1-2H3
InchiKey: APRDSJRFFKMSPY-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC1CCC2=C(C1)OC(=O)C2C
Mol. weight [g/mol]: 166.22
CAS: 16642-41-4

Physical Properties

Property code	Value	Unit	Source
hfus	20.64	kJ/mol	Joback Method
logp	2.253		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
rinpol	1353.80		NIST Webbook
tb	522.47	K	Cheméo Relay (1.0)
tf	349.32	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-5.00200e+01
Coeff. B	1.01624e+00
Coeff. C	-6.72800e-04
Coeff. D	1.73800e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc

Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-8.56069e+00
Coeff. B	6.25170e+02
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	302.95
Temperature range (K), max.	504.59

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16642414&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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