Methyl (4S,5R)-2,2,5-trimethyl-1,3-dioxolane-4-carboxylat

Inchi: InChI=1S/C8H14O4/c1-5-6(7(9)10-4)12-8(2,3)11-5/h5-6H,1-4H3
InchiKey: AELKYRWKHKGMAD-UHFFFAOYSA-N
Formula: C8H14O4
SMILES: COC(=O)C1OC(C)(C)OC1C
Mol. weight [g/mol]: 174.19
CAS: 38410-80-9

Physical Properties

Property code	Value	Unit	Source
gf	-374.04	kJ/mol	Joback Method
hf	-682.21	kJ/mol	Joback Method
hfus	25.00	kJ/mol	Joback Method
hvap	50.07	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	0.699		Crippen Method
mcvol	131.900	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1037.50		NIST Webbook
tb	518.81	K	Joback Method
tc	728.24	K	Joback Method
tf	331.54	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.15	J/mol×K	518.81	Joback Method
cpg	340.84	J/mol×K	553.72	Joback Method
cpg	354.72	J/mol×K	588.62	Joback Method
cpg	367.87	J/mol×K	623.53	Joback Method
cpg	380.36	J/mol×K	658.43	Joback Method
cpg	392.25	J/mol×K	693.34	Joback Method
cpg	403.63	J/mol×K	728.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38410809&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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