[(E)-3,3-dimethylcyclohexylidene] methyl formate

Inchi: InChI=1S/C10H16O2/c1-10(2)5-3-4-9(6-10)7-12-8-11/h7-8H,3-6H2,1-2H3/b9-7+

InchiKey: FWZOZUXJYAXNBJ-VQHVLOKHSA-N

Formula: C10H16O2

SMILES: CC1(C)CCCC(=COC=O)C1

Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-106.78	kJ/mol	Joback Method
hf	-321.94	kJ/mol	Joback Method
hfus	10.99	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.643		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1210.00		NIST Webbook
tb	525.71	K	Joback Method
tc	741.39	K	Joback Method
tf	308.33	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.10	J/mol×K	525.71	Joback Method
cpg	354.28	J/mol×K	561.66	Joback Method
cpg	369.48	J/mol×K	597.60	Joback Method
cpg	383.81	J/mol×K	633.55	Joback Method
cpg	397.36	J/mol×K	669.49	Joback Method
cpg	410.22	J/mol×K	705.44	Joback Method
cpg	422.51	J/mol×K	741.39	Joback Method

Sources

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=R216434&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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