Cubane-1,4-dicarboylic acid dimethyl ester

Inchi: InChI=1S/C12H12O4/c1-15-9(13)11-3-6-4(11)8-5(11)7(3)12(6,8)10(14)16-2/h3-8H,1-2H3
InchiKey: OXBMFCGRQJNAOY-UHFFFAOYSA-N
Formula: C12H12O4
SMILES: COC(=O)C12C3C4C1C1C2C3C41C(=O)OC
Mol. weight [g/mol]: 220.22
CAS: 29412-62-2

Physical Properties

Property code	Value	Unit	Source
chs	-6218.10 ± 1.40	kJ/mol	NIST Webbook
gf	-63.34	kJ/mol	Joback Method
hf	-404.03	kJ/mol	Joback Method
hfs	-219.00 ± 2.10	kJ/mol	NIST Webbook
hfus	28.40	kJ/mol	Joback Method
hsub	118.90 ± 3.80	kJ/mol	NIST Webbook
hsub	117.20 ± 3.90	kJ/mol	NIST Webbook
hvap	88.50 ± 2.20	kJ/mol	NIST Webbook
log10ws	-0.11		Crippen Method
logp	0.070		Crippen Method
mcvol	140.520	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	616.82	K	Joback Method
tc	825.08	K	Joback Method
tf	437.80 ± 0.50	K	NIST Webbook
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.48	J/mol×K	651.53	Joback Method
cpg	455.67	J/mol×K	686.24	Joback Method
cpg	466.42	J/mol×K	720.95	Joback Method
cpg	477.05	J/mol×K	755.66	Joback Method
cpg	487.85	J/mol×K	790.37	Joback Method

cpg	432.55	J/mol×K	616.82	Joback Method
cpg	499.14	J/mol×K	825.08	Joback Method
cps	251.10	J/mol×K	298.15	NIST Webbook
hfust	41.00	kJ/mol	437.80	NIST Webbook
hfust	38.10	kJ/mol	438.20	NIST Webbook
hfust	41.00	kJ/mol	437.80	NIST Webbook
sfust	93.70	J/mol×K	437.80	NIST Webbook

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=C29412622&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation 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
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume