

3,4-Dimethoxy adipic acid, dimethyl ester

Inchi:	InChI=1S/C10H18O6/c1-13-7(5-9(11)15-3)8(14-2)6-10(12)16-4/h7-8H,5-6H2,1-4H3
InchiKey:	WUWLMYNLJRZTOV-UHFFFAOYSA-N
Formula:	C10H18O6
SMILES:	COC(=O)CC(OC)C(CC(=O)OC)OC
Mol. weight [g/mol]:	234.25

Physical Properties

Property code	Value	Unit	Source
gf	-649.40	kJ/mol	Joback Method
hf	-1014.33	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-0.13		Crippen Method
logp	0.143		Crippen Method
mcvol	178.380	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
tb	624.74	K	Joback Method
tc	809.53	K	Joback Method
tf	361.24	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.07	J/molxK	624.74	Joback Method
cpg	481.58	J/molxK	655.54	Joback Method
cpg	494.52	J/molxK	686.34	Joback Method
cpg	506.86	J/molxK	717.13	Joback Method
cpg	518.58	J/molxK	747.93	Joback Method
cpg	529.66	J/molxK	778.73	Joback Method
cpg	540.07	J/molxK	809.53	Joback Method
dvisc	0.0015044	Paxs	361.24	Joback Method
dvisc	0.0007526	Paxs	405.16	Joback Method
dvisc	0.0004311	Paxs	449.07	Joback Method

dvisc	0.0002727	Paxs	492.99	Joback Method
dvisc	0.0001859	Paxs	536.91	Joback Method
dvisc	0.0001343	Paxs	580.82	Joback Method
dvisc	0.0001016	Paxs	624.74	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=B6000978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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