

Dimethyl 2,2'-dibromoadipate

Inchi:	InChI=1S/C8H12Br2O4/c1-13-7(11)5(9)3-4-6(10)8(12)14-2/h5-6H,3-4H2,1-2H3
InchiKey:	HVICCJCVLLCDFQ-UHFFFAOYSA-N
Formula:	C8H12Br2O4
SMILES:	COC(=O)C(Br)CCC(Br)C(=O)OC
Mol. weight [g/mol]:	331.99
CAS:	868-72-4

Physical Properties

Property code	Value	Unit	Source
gf	-427.60	kJ/mol	Joback Method
hf	-655.95	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	63.81	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.640		Crippen Method
mcvol	173.460	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	666.46	K	Joback Method
tc	882.09	K	Joback Method
tf	413.84	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.82	J/molxK	666.46	Joback Method
cpg	404.26	J/molxK	702.40	Joback Method
cpg	414.04	J/molxK	738.34	Joback Method
cpg	423.18	J/molxK	774.27	Joback Method
cpg	431.69	J/molxK	810.21	Joback Method
cpg	439.57	J/molxK	846.15	Joback Method
cpg	446.82	J/molxK	882.09	Joback Method
dvisc	0.0015070	Paxs	413.84	Joback Method
dvisc	0.0008732	Paxs	455.94	Joback Method

dvisc	0.0005549	Paxs	498.05	Joback Method
dvisc	0.0003784	Paxs	540.15	Joback Method
dvisc	0.0002728	Paxs	582.25	Joback Method
dvisc	0.0002055	Paxs	624.36	Joback Method
dvisc	0.0001604	Paxs	666.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C868724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
mccvol:	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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