

BENZALMALONIC DIALDEHYDE

Other names:	Benzalmalonic dialdehyde
Inchi:	InChI=1S/C10H8O2/c11-7-10(8-12)6-9-4-2-1-3-5-9/h1-8H
InchiKey:	XXUUYXIFVYQLKJ-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	O=CC(C=O)=Cc1cccc1
Mol. weight [g/mol]:	160.17

Physical Properties

Property code	Value	Unit	Source
af	0.4777		Cheméo Relay (1.0)
gf	18.36	kJ/mol	Joback Method
hf	-54.71	kJ/mol	Cheméo Relay (1.0)
hfus	19.17	kJ/mol	Joback Method
hvap	57.53	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-2.07		Cheméo Relay (1.0)
logp	1.468		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	536.11	K	Cheméo Relay (1.0)
tc	785.65	K	Cheméo Relay (1.0)
tf	308.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.95	J/mol×K	556.24	Joback Method
cpg	287.44	J/mol×K	594.10	Joback Method
cpg	298.06	J/mol×K	631.97	Joback Method
cpg	307.86	J/mol×K	669.83	Joback Method
cpg	316.90	J/mol×K	707.70	Joback Method
cpg	325.24	J/mol×K	745.56	Joback Method
cpg	332.93	J/mol×K	783.43	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C82700434&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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