DIETHYL METHYLSUCCINATE

Other names: Butanedioic acid, methyl-, diethyl ester
Diethyl methylbutanedioate
Inchi: InChI=1S/C9H16O4/c1-4-12-8(10)6-7(3)9(11)13-5-2/h7H,4-6H2,1-3H3
InchiKey: XHLXMRJWRKQMCP-UHFFFAOYSA-N
Formula: C9H16O4
SMILES: CCOC(=O)CC(C)C(=O)OCC
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
af	0.5799		Cheméo Relay (1.0)
gf	-445.38	kJ/mol	Joback Method
hf	-873.65	kJ/mol	Cheméo Relay (1.0)
hfus	21.12	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-1.50		Cheméo Relay (1.0)
logp	1.139		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1205.00		NIST Webbook
rinpol	1205.00		NIST Webbook
tb	466.32	K	Cheméo Relay (1.0)
tc	655.09	K	Cheméo Relay (1.0)
tf	239.47	K	Cheméo Relay (1.0)
vc	0.577	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.40	J/mol×K	557.46	Joback Method
cpg	436.72	J/mol×K	742.78	Joback Method
cpg	426.64	J/mol×K	711.90	Joback Method
cpg	416.03	J/mol×K	681.01	Joback Method

cpg	404.90	J/mol×K	650.12	Joback Method
cpg	393.25	J/mol×K	619.23	Joback Method
cpg	381.08	J/mol×K	588.35	Joback Method
dvisc	0.0004996	Pa×s	438.99	Joback Method
dvisc	0.0001960	Pa×s	557.46	Joback Method
dvisc	0.0002553	Pa×s	517.97	Joback Method
dvisc	0.0003474	Pa×s	478.48	Joback Method
dvisc	0.0025423	Pa×s	320.51	Joback Method
dvisc	0.0007719	Pa×s	399.49	Joback Method
dvisc	0.0013123	Pa×s	360.00	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4676511&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

Legend

af: Acentric Factor
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
ie: Ionization energy
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