

Diallyl succinate

Other names:	Butanedioic acid, di-2-propenyl ester JF 2777 JF 3958 Succinic acid, diallyl ester
Inchi:	InChI=1S/C10H14O4/c1-3-7-13-9(11)5-6-10(12)14-8-4-2/h3-4H,1-2,5-8H2
InchiKey:	HABAXTXIECRCKH-UHFFFAOYSA-N
Formula:	C10H14O4
SMILES:	<chem>C=CCOC(=O)CCC(=O)OCC=C</chem>
Mol. weight [g/mol]:	198.22
CAS:	925-16-6

Physical Properties

Property code	Value	Unit	Source
gf	-258.84	kJ/mol	Joback Method
hf	-488.47	kJ/mol	Joback Method
hfus	24.67	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.225		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
tb	574.14	K	Joback Method
tc	760.60	K	Joback Method
tf	343.26	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.22	J/mol×K	574.14	Joback Method
cpg	387.19	J/mol×K	605.22	Joback Method
cpg	398.63	J/mol×K	636.29	Joback Method

cpg	409.53	J/molxK	667.37	Joback Method
cpg	419.89	J/molxK	698.44	Joback Method
cpg	429.73	J/molxK	729.52	Joback Method
cpg	439.03	J/molxK	760.60	Joback Method
dvisc	0.0017838	Paxs	343.26	Joback Method
dvisc	0.0010336	Paxs	381.74	Joback Method
dvisc	0.0006618	Paxs	420.22	Joback Method
dvisc	0.0004567	Paxs	458.70	Joback Method
dvisc	0.0003338	Paxs	497.18	Joback Method
dvisc	0.0002552	Paxs	535.66	Joback Method
dvisc	0.0002023	Paxs	574.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	0.40	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C925166&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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