Hexanedioic acid, di-2-propenyl ester

Other names:	Adipic acid, diallyl ester
	Allyl adipate
	Diallyl adipate
	Diallylester kyseliny adipove
	Hexanedioic acid, bis(2-propenyl) ester
	Diallyl hexanedioate
Inchi:	InChI=1S/C12H18O4/c1-3-9-15-11(13)7-5-6-8-12(14)16-10-4-2/h3-4H,1-2,5-10H2
InchiKey:	FPODCVUTIPDRTE-UHFFFAOYSA-N
Formula:	C12H18O4
SMILES:	C=CCOC(=O)CCCCC(=O)OCC=C
Mol. weight [g/mol]:	226.27
CAS:	2998-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-242.00	kJ/mol	Joback Method
hf	-529.75	kJ/mol	Joback Method
hfus	29.85	kJ/mol	Joback Method
hvap	59.28	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.005		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1567.00		NIST Webbook
tb	619.90	K	Joback Method
tc	802.73	K	Joback Method
tf	365.80	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	472.49	J/mol×K	619.90	Joback Method
cpg	533.37	J/mol×K	772.26	Joback Method
cpg	522.43	J/mol×K	741.78	Joback Method
cpg	510.88	J/mol×K	711.31	Joback Method
cpg	498.71	J/mol×K	680.84	Joback Method
cpg	485.91	J/mol×K	650.37	Joback Method
cpg	543.71	J/mol×K	802.73	Joback Method
dvisc	0.0001655	Pa×s	619.90	Joback Method
dvisc	0.0002108	Pa×s	577.55	Joback Method
dvisc	0.0002790	Pa×s	535.20	Joback Method
dvisc	0.0003875	Pa×s	492.85	Joback Method
dvisc	0.0005726	Pa×s	450.50	Joback Method
dvisc	0.0009174	Pa×s	408.15	Joback Method
dvisc	0.0016394	Pa×s	365.80	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2998041&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume