1,3-butanediol diacrylate

Other names: 2-propenoic acid 1-methyl-1,3-propanediyl ester
butane-1,3-diyl diacrylate
Inchi: InChI=1S/C10H14O4/c1-4-9(11)13-7-6-8(3)14-10(12)5-2/h4-5,8H,1-2,6-7H2,3H3
InchiKey: FQMIAEWUVYWVNB-UHFFFAOYSA-N
Formula: C10H14O4
SMILES: C=CC(=O)OCCC(C)OC(=O)C=C
Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
af	0.6440		Cheméo Relay (1.0)
hf	-669.31	kJ/mol	Cheméo Relay (1.0)
hfus	21.15	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Cheméo Relay (1.0)
ie	10.11	eV	Cheméo Relay (1.0)
log10ws	-1.85		Cheméo Relay (1.0)
logp	1.223		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
tb	488.57	K	Cheméo Relay (1.0)
tc	679.61	K	Cheméo Relay (1.0)
tf	248.62	K	Cheméo Relay (1.0)
vc	0.572	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.61	J/mol×K	573.70	Joback Method
cpg	440.69	J/mol×K	763.74	Joback Method
cpg	431.25	J/mol×K	732.07	Joback Method
cpg	421.25	J/mol×K	700.40	Joback Method
cpg	410.69	J/mol×K	668.72	Joback Method
cpg	399.56	J/mol×K	637.05	Joback Method
cpg	387.87	J/mol×K	605.37	Joback Method

dvisc	0.0004656	Pa×s	450.98	Joback Method
dvisc	0.0001894	Pa×s	573.70	Joback Method
dvisc	0.0002441	Pa×s	532.79	Joback Method
dvisc	0.0003282	Pa×s	491.89	Joback Method
dvisc	0.0022419	Pa×s	328.26	Joback Method
dvisc	0.0007082	Pa×s	410.07	Joback Method
dvisc	0.0011821	Pa×s	369.17	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Phase behaviour for the (carbon dioxide + 1,3-butanediol diacrylate) and (carbon dioxide + 1,3-butanediol dimethacrylate) systems at elevated pressures and temperatures: https://www.doi.org/10.1016/j.jct.2013.11.030

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
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
vc: Critical Volume