Diethyl 2-(But-3-enyl)propanedioate

Inchi: InChI=1S/C12H20O4/c1-4-7-8-10(11(13)15-6-3)12(14)16-9-5-2/h4,10H,1,5-9H2,2-3H3
InchiKey: YZOLINQKIXIFPE-UHFFFAOYSA-N
Formula: C12H20O4
SMILES: C=CCCC(C(=O)OCC)C(=O)OCCC
Mol. weight [g/mol]: 228.28

Physical Properties

Property code	Value	Unit	Source
gf	-332.28	kJ/mol	Joback Method
hf	-660.46	kJ/mol	Joback Method
hfus	27.61	kJ/mol	Joback Method
hvap	59.56	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.085		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1338.00		NIST Webbook
rinpol	1338.00		NIST Webbook
tb	622.78	K	Joback Method
tc	805.80	K	Joback Method
tf	352.56	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.56	J/mol×K	622.78	Joback Method
cpg	508.83	J/mol×K	653.28	Joback Method
cpg	522.44	J/mol×K	683.79	Joback Method
cpg	535.40	J/mol×K	714.29	Joback Method
cpg	547.70	J/mol×K	744.79	Joback Method
cpg	559.35	J/mol×K	775.29	Joback Method
cpg	570.35	J/mol×K	805.80	Joback Method
dvisc	0.0020843	Pa×s	352.56	Joback Method

dvisc	0.0010448	Pa×s	397.60	Joback Method
dvisc	0.0006027	Pa×s	442.63	Joback Method
dvisc	0.0003849	Pa×s	487.67	Joback Method
dvisc	0.0002652	Pa×s	532.71	Joback Method
dvisc	0.0001936	Pa×s	577.74	Joback Method
dvisc	0.0001479	Pa×s	622.78	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R508986&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume