Ethanedioic acid, bis(3-methylbutyl) ester

Other names: Di-iso-amyl oxalate
diisopentyl oxalate
Inchi: InChI=1S/C12H22O4/c1-9(2)5-7-15-11(13)12(14)16-8-6-10(3)4/h9-10H,5-8H2,1-4H3
InchiKey: HCUOPEBHVAVNIE-UHFFFAOYSA-N
Formula: C12H22O4
SMILES: CC(C)CCOC(=O)C(=O)OCCC(C)C
Mol. weight [g/mol]: 230.30
CAS: 2051-00-5

Physical Properties

Property code	Value	Unit	Source
gf	-422.56	kJ/mol	Joback Method
hf	-791.17	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.165		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
tb	625.66	K	Joback Method
tc	808.87	K	Joback Method
tf	339.32	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.13	J/mol×K	808.87	Joback Method
cpg	585.47	J/mol×K	778.33	Joback Method
cpg	573.11	J/mol×K	747.80	Joback Method
cpg	560.07	J/mol×K	717.26	Joback Method
cpg	546.34	J/mol×K	686.73	Joback Method

cpg	531.92	J/mol×K	656.19	Joback Method
cpg	516.81	J/mol×K	625.66	Joback Method
dvisc	0.0027555	Pa×s	339.32	Joback Method
dvisc	0.0001321	Pa×s	625.66	Joback Method
dvisc	0.0001778	Pa×s	577.94	Joback Method
dvisc	0.0002525	Pa×s	530.21	Joback Method
dvisc	0.0003843	Pa×s	482.49	Joback Method
dvisc	0.0006416	Pa×s	434.77	Joback Method
dvisc	0.0012154	Pa×s	387.04	Joback Method
hvapt	58.60	kJ/mol	448.00	NIST Webbook

Sources

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=C2051005&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt: Enthalpy of vaporization at a given temperature
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