Malonic acid, 2-ethylbutyl pentyl ester

Inchi: InChI=1S/C14H26O4/c1-4-7-8-9-17-13(15)10-14(16)18-11-12(5-2)6-3/h12H,4-11H2,1-3H
InchiKey: RSQAXPIBCULDMW-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCCCOC(=O)CC(=O)OCC(CC)CC
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-403.28	kJ/mol	Joback Method
hf	-827.17	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.089		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1690.00		NIST Webbook
tb	671.86	K	Joback Method
tc	850.20	K	Joback Method
tf	376.86	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.64	J/mol×K	671.86	Joback Method
cpg	638.53	J/mol×K	701.58	Joback Method
cpg	653.66	J/mol×K	731.31	Joback Method
cpg	668.05	J/mol×K	761.03	Joback Method
cpg	681.70	J/mol×K	790.75	Joback Method
cpg	694.61	J/mol×K	820.48	Joback Method
cpg	706.79	J/mol×K	850.20	Joback Method
dvisc	0.0018269	Pa×s	376.86	Joback Method
dvisc	0.0008752	Pa×s	426.03	Joback Method

dvisc	0.0004883	Pa×s	475.19	Joback Method
dvisc	0.0003039	Pa×s	524.36	Joback Method
dvisc	0.0002052	Pa×s	573.53	Joback Method
dvisc	0.0001474	Pa×s	622.69	Joback Method
dvisc	0.0001111	Pa×s	671.86	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=U348955&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