Malonic acid, hexyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C15H28O4/c1-5-6-7-8-9-18-14(16)11-15(17)19-13(4)10-12(2)3/h12-13H,5-11H
InchiKey: ONTOEBPJPHFONQ-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCCCCOC(=O)CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-397.30	kJ/mol	Joback Method
hf	-853.09	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.478		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	694.30	K	Joback Method
tc	874.56	K	Joback Method
tf	373.13	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.23	J/mol×K	694.30	Joback Method
cpg	752.95	J/mol×K	844.52	Joback Method
cpg	739.62	J/mol×K	814.47	Joback Method
cpg	725.49	J/mol×K	784.43	Joback Method
cpg	710.56	J/mol×K	754.39	Joback Method
cpg	694.81	J/mol×K	724.34	Joback Method
cpg	765.47	J/mol×K	874.56	Joback Method
dvisc	0.0000905	Pa×s	694.30	Joback Method

dvisc	0.0001227	Pa×s	640.77	Joback Method
dvisc	0.0001760	Pa×s	587.24	Joback Method
dvisc	0.0002714	Pa×s	533.71	Joback Method
dvisc	0.0004608	Pa×s	480.19	Joback Method
dvisc	0.0008937	Pa×s	426.66	Joback Method
dvisc	0.0020958	Pa×s	373.13	Joback Method

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=U349335&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
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