Malonic acid, 3,3-dimethylbut-2-yl undecyl ester

Inchi: InChI=1S/C20H38O4/c1-6-7-8-9-10-11-12-13-14-15-23-18(21)16-19(22)24-17(2)20(3,4)5

InchiKey: PDXGBLBIBPMVBJ-UHFFFAOYSA-N

Formula: C20H38O4

SMILES: CCCCCCCCCCCOC(=O)CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-349.92	kJ/mol	Joback Method
hf	-959.76	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	76.74	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.428		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	805.91	K	Joback Method
tc	992.86	K	Joback Method
tf	446.90	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.67	J/mol×K	805.91	Joback Method
cpg	1051.98	J/mol×K	961.70	Joback Method
cpg	1037.73	J/mol×K	930.54	Joback Method
cpg	1022.51	J/mol×K	899.38	Joback Method
cpg	1006.28	J/mol×K	868.23	Joback Method
cpg	989.01	J/mol×K	837.07	Joback Method
cpg	1065.27	J/mol×K	992.86	Joback Method
dvisc	0.0000392	Pa×s	805.91	Joback Method

dvisc	0.0000540	Pa×s	746.08	Joback Method
dvisc	0.0000785	Pa×s	686.24	Joback Method
dvisc	0.0001227	Pa×s	626.40	Joback Method
dvisc	0.0002108	Pa×s	566.57	Joback Method
dvisc	0.0004114	Pa×s	506.73	Joback Method
dvisc	0.0009605	Pa×s	446.90	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=U348662&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