Malonic acid, 2-methylpentyl undecyl ester

Inchi: InChI=1S/C20H38O4/c1-4-6-7-8-9-10-11-12-13-15-23-19(21)16-20(22)24-17-18(3)14-5-2
InchiKey: YMIDJZBIDXUYAM-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: CCCCCCCCCCCOC(=O)CC(=O)OCC(C)CCC
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-352.76	kJ/mol	Joback Method
hf	-951.01	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.430		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2203.00		NIST Webbook
tb	809.14	K	Joback Method
tc	993.61	K	Joback Method
tf	444.48	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.66	J/mol×K	809.14	Joback Method
cpg	987.99	J/mol×K	839.88	Joback Method
cpg	1005.26	J/mol×K	870.63	Joback Method
cpg	1021.49	J/mol×K	901.37	Joback Method
cpg	1036.69	J/mol×K	932.12	Joback Method
cpg	1050.89	J/mol×K	962.86	Joback Method
cpg	1064.10	J/mol×K	993.61	Joback Method
dvisc	0.0009916	Pa×s	444.48	Joback Method
dvisc	0.0004441	Pa×s	505.26	Joback Method

dvisc	0.0002364	Pa×s	566.03	Joback Method
dvisc	0.0001422	Pa×s	626.81	Joback Method
dvisc	0.0000935	Pa×s	687.59	Joback Method
dvisc	0.0000659	Pa×s	748.36	Joback Method
dvisc	0.0000489	Pa×s	809.14	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=U349303&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

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