2,4,4-Trimethylpentane-1,3-diyl bis(2-methylpropanoate)

Inchi: InChI=1S/C16H30O4/c1-11(2)14(17)19-9-13(5)8-16(6,7)10-20-15(18)12(3)4/h11-13H,8-1

InchiKey: GVZLNOOLGIOOEC-UHFFFAOYSA-N

Formula: C16H30O4

SMILES: CC(COC(=O)C(C)C)CC(C)(C)COC(=O)C(C)C

Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-388.48	kJ/mol	Joback Method
hf	-887.76	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	67.06	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.437		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	1572.00		NIST Webbook
tb	713.51	K	Joback Method
tc	902.39	K	Joback Method
tf	371.82	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.13	J/mol×K	713.51	Joback Method
cpg	754.71	J/mol×K	744.99	Joback Method
cpg	771.31	J/mol×K	776.47	Joback Method
cpg	786.95	J/mol×K	807.95	Joback Method
cpg	801.66	J/mol×K	839.43	Joback Method
cpg	815.44	J/mol×K	870.91	Joback Method
cpg	828.34	J/mol×K	902.39	Joback Method
dvisc	0.0025831	Pa×s	371.82	Joback Method
dvisc	0.0009143	Pa×s	428.77	Joback Method

dvisc	0.0004128	Pa×s	485.72	Joback Method
dvisc	0.0002203	Pa×s	542.66	Joback Method
dvisc	0.0001324	Pa×s	599.61	Joback Method
dvisc	0.0000870	Pa×s	656.56	Joback Method
dvisc	0.0000611	Pa×s	713.51	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=R519496&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