

Propane-1,2-diyl bis((E)-2-methylbut-2-enoate)

Inchi:	InChI=1S/C13H20O4/c1-6-9(3)12(14)16-8-11(5)17-13(15)10(4)7-2/h6-7,11H,8H2,1-5H3/
InchiKey:	DILQUQINCSKBIG-KZZDLZNXSA-N
Formula:	C13H20O4
SMILES:	CC=C(C)C(=O)OCC(C)OC(=O)C(C)=CC
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	-268.36	kJ/mol	Joback Method
hf	-591.67	kJ/mol	Joback Method
hfus	29.26	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.394		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinsol	1628.00		NIST Webbook
tb	657.06	K	Joback Method
tc	854.07	K	Joback Method
tf	327.51	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.05	J/mol×K	657.06	Joback Method
cpg	539.82	J/mol×K	689.90	Joback Method
cpg	553.79	J/mol×K	722.73	Joback Method
cpg	567.01	J/mol×K	755.57	Joback Method
cpg	579.49	J/mol×K	788.40	Joback Method
cpg	591.26	J/mol×K	821.24	Joback Method
cpg	602.34	J/mol×K	854.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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