

Propane-1,3-diyl bis((E)-2-methylbut-2-enoate)

Inchi:	InChI=1S/C13H20O4/c1-5-10(3)12(14)16-8-7-9-17-13(15)11(4)6-2/h5-6H,7-9H2,1-4H3/b
InchiKey:	CUYYUCBNBIAVDR-YOYBCKCWSA-N
Formula:	C13H20O4
SMILES:	CC=C(C)C(=O)OCCOC(=O)C(C)=CC
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	-265.92	kJ/mol	Joback Method
hf	-586.39	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	62.92	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.395		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinqol	1745.00		NIST Webbook
tb	657.50	K	Joback Method
tc	851.18	K	Joback Method
tf	342.51	K	Joback Method
vc	0.773	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.57	J/molxK	657.50	Joback Method
cpg	539.05	J/molxK	689.78	Joback Method
cpg	552.78	J/molxK	722.06	Joback Method
cpg	565.78	J/molxK	754.34	Joback Method
cpg	578.08	J/molxK	786.62	Joback Method
cpg	589.70	J/molxK	818.90	Joback Method
cpg	600.66	J/molxK	851.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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