

Succinic acid, di(3-methylbut-3-enyl) ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H22O4/c1-11(2)7-9-17-13(15)5-6-14(16)18-10-8-12(3)4/h1,3,5-10H2,2,4H3

PPUPRAXYBKCKDU-UHFFFAOYSA-N

C14H22O4

C=C(C)CCOC(=O)CCC(=O)OCCC(=C)C

254.32

Physical Properties

Property code	Value	Unit	Source
gf	-242.26	kJ/mol	Joback Method
hf	-590.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.785		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1715.00		NIST Webbook
tb	665.42	K	Joback Method
tc	850.41	K	Joback Method
tf	360.42	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.29	J/mol×K	665.42	Joback Method
cpg	590.19	J/mol×K	696.25	Joback Method
cpg	604.34	J/mol×K	727.08	Joback Method
cpg	617.77	J/mol×K	757.91	Joback Method
cpg	630.47	J/mol×K	788.75	Joback Method
cpg	642.46	J/mol×K	819.58	Joback Method
cpg	653.76	J/mol×K	850.41	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353456&Units=SI

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
hvac:	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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