

Succinic acid, 3-methylbut-2-en-1-yl trans-hex-3-en-1-yl ester

Inchi:	InChI=1S/C15H24O4/c1-4-5-6-7-11-18-14(16)8-9-15(17)19-12-10-13(2)3/h5-6,10H,4,7-9
InchiKey:	MJVG YAWABWDYLV-AATRIKPKSA-N
Formula:	C15H24O4
SMILES:	CCC=CCCOC(=O)CCC(=O)OCC=C(C)C
Mol. weight [g/mol]:	268.35

Physical Properties

Property code	Value	Unit	Source
gf	-240.53	kJ/mol	Joback Method
hf	-617.88	kJ/mol	Joback Method
hfus	39.27	kJ/mol	Joback Method
hvap	67.29	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.175		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinsol	1845.00		NIST Webbook
tb	703.38	K	Joback Method
tc	891.50	K	Joback Method
tf	379.01	K	Joback Method
vc	0.884	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.46	J/mol×K	703.38	Joback Method
cpg	646.74	J/mol×K	734.73	Joback Method
cpg	661.22	J/mol×K	766.09	Joback Method
cpg	674.93	J/mol×K	797.44	Joback Method
cpg	687.91	J/mol×K	828.79	Joback Method
cpg	700.17	J/mol×K	860.15	Joback Method
cpg	711.74	J/mol×K	891.50	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=U391113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
mccvol:	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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