

Succinic acid, 3-methylbut-2-yl hept-1,6-dien-4-yl ester

Inchi:	InChI=1S/C16H26O4/c1-6-8-14(9-7-2)20-16(18)11-10-15(17)19-13(5)12(3)4/h6-7,12-14H
InchiKey:	BZIYFCWUMUOUCX-UHFFFAOYSA-N
Formula:	C16H26O4
SMILES:	C=CCC(CC=C)OC(=O)CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	282.38

Physical Properties

Property code	Value	Unit	Source
gf	-215.64	kJ/mol	Joback Method
hf	-628.15	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.418		Crippen Method
mvol	242.580	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	710.10	K	Joback Method
tc	896.56	K	Joback Method
tf	365.88	K	Joback Method
vc	0.923	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.11	J/molxK	710.10	Joback Method
cpg	702.29	J/molxK	741.18	Joback Method
cpg	717.59	J/molxK	772.25	Joback Method
cpg	732.03	J/molxK	803.33	Joback Method
cpg	745.62	J/molxK	834.40	Joback Method
cpg	758.39	J/molxK	865.48	Joback Method
cpg	770.33	J/molxK	896.56	Joback Method
dvisc	0.0023541	Paxs	365.88	Joback Method

dvisc	0.0009198	Paxs	423.25	Joback Method
dvisc	0.0004498	Paxs	480.62	Joback Method
dvisc	0.0002562	Paxs	537.99	Joback Method
dvisc	0.0001626	Paxs	595.36	Joback Method
dvisc	0.0001118	Paxs	652.73	Joback Method
dvisc	0.0000817	Paxs	710.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391329&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/92-575-2/Succinic-acid-3-methylbut-2-yl-hept-1-6-dien-4-yl-ester.pdf>

Generated by Cheméo on 2024-04-29 10:00:59.162848346 +0000 UTC m=+16674108.083425661.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.