

Succinic acid, di(trans-hex-3-enyl) ester

Inchi: InChI=1S/C16H26O4/c1-3-5-7-9-13-19-15(17)11-12-16(18)20-14-10-8-6-4-2/h5-8H,3-4,9
InchiKey: MPKJFHUGBKINTM-KQQUZDAGSA-N
Formula: C16H26O4
SMILES: CCC=CCCOC(=O)CCC(=O)OCCC=CCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-223.56	kJ/mol	Joback Method
hf	-628.73	kJ/mol	Joback Method
hfus	43.17	kJ/mol	Joback Method
hvap	69.44	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mvol	242.580	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	726.38	K	Joback Method
tc	911.77	K	Joback Method
tf	404.24	K	Joback Method
vc	0.940	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.97	J/molxK	726.38	Joback Method
cpg	756.90	J/molxK	880.87	Joback Method
cpg	744.43	J/molxK	849.97	Joback Method
cpg	731.22	J/molxK	819.07	Joback Method
cpg	717.26	J/molxK	788.18	Joback Method
cpg	702.52	J/molxK	757.28	Joback Method
cpg	768.68	J/molxK	911.77	Joback Method
dvisc	0.0000692	Paxs	726.38	Joback Method

dvisc	0.0000911	Paxs	672.69	Joback Method
dvisc	0.0001259	Paxs	619.00	Joback Method
dvisc	0.0001849	Paxs	565.31	Joback Method
dvisc	0.0002944	Paxs	511.62	Joback Method
dvisc	0.0005229	Paxs	457.93	Joback Method
dvisc	0.0010816	Paxs	404.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353437&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
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

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