

Succinic acid, 2-methylpent-3-yl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C17H30O4/c1-5-15(12(2)3)21-17(19)11-10-16(18)20-14-8-6-13(4)7-9-14/h12-14,16-17,19-21
InchiKey: PDRWEHXQZVZRDF-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: CCC(OC(=O)CCC(=O)OC1CCC(C)CC1)C(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-363.72	kJ/mol	Joback Method
hf	-860.39	kJ/mol	Joback Method
hfus	31.22	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.866		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	754.94	K	Joback Method
tc	955.18	K	Joback Method
tf	398.81	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.61	J/molxK	754.94	Joback Method
cpg	875.23	J/molxK	921.80	Joback Method
cpg	860.80	J/molxK	888.43	Joback Method
cpg	845.14	J/molxK	855.06	Joback Method
cpg	828.22	J/molxK	821.69	Joback Method
cpg	810.05	J/molxK	788.31	Joback Method
cpg	888.42	J/molxK	955.18	Joback Method
dvisc	0.0000896	Paxs	754.94	Joback Method

dvisc	0.0001202	Paxs	695.59	Joback Method
dvisc	0.0001703	Paxs	636.23	Joback Method
dvisc	0.0002593	Paxs	576.88	Joback Method
dvisc	0.0004348	Paxs	517.52	Joback Method
dvisc	0.0008336	Paxs	458.17	Joback Method
dvisc	0.0019397	Paxs	398.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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