Succinic acid, di(4-methylhept-3-yl) ester

Inchi: InChI=1S/C21H40O4/c1-7-11-16(5)18(10-4)24-20(22)14-15-21(23)25-19(13-9-3)17(6)12
InchiKey: YKVSIRQKAOPYIK-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCC(C)C(CC)OC(=O)CCC(=O)OC(CCC)C(C)CCC
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-351.66	kJ/mol	Joback Method
hf	-987.49	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	79.10	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.673		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
tb	830.70	K	Joback Method
tc	1020.47	K	Joback Method
tf	410.75	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.14	J/mol×K	830.70	Joback Method
cpg	1115.14	J/mol×K	988.84	Joback Method
cpg	1100.82	J/mol×K	957.21	Joback Method
cpg	1085.37	J/mol×K	925.58	Joback Method
cpg	1068.79	J/mol×K	893.96	Joback Method
cpg	1051.06	J/mol×K	862.33	Joback Method
cpg	1128.36	J/mol×K	1020.47	Joback Method
dvisc	0.0000326	Pa×s	830.70	Joback Method

dvisc	0.0000463	Pa×s	760.71	Joback Method
dvisc	0.0000707	Pa×s	690.72	Joback Method
dvisc	0.0001187	Pa×s	620.73	Joback Method
dvisc	0.0002275	Pa×s	550.73	Joback Method
dvisc	0.0005267	Pa×s	480.74	Joback Method
dvisc	0.0016234	Pa×s	410.75	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381358&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/80-183-0/Succinic-acid-di-4-methylhept-3-yl-ester.pdf
Generated by Cheméo on 2024-04-25 19:05:37.817765708 +0000 UTC m=+16361186.738343023.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.