Succinic acid, hept-2-yl adamant-2-yl ester

Inchi: InChI=1S/C21H34O4/c1-3-4-5-6-14(2)24-19(22)7-8-20(23)25-21-17-10-15-9-16(12-17)13
InchiKey: BYLKFEZAWZSJKZ-UHFFFAOYSA-N
Formula: C21H34O4
SMILES: CCCCCC(C)OC(=O)CCC(=O)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-189.61	kJ/mol	Joback Method
hf	-800.09	kJ/mol	Joback Method
hfus	46.64	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.647		Crippen Method
mcvol	289.050	ml/mol	McGowan Method
pc	1289.29	kPa	Joback Method
rinpol	2554.00		NIST Webbook
rinpol	2554.00		NIST Webbook
tb	847.17	K	Joback Method
tc	1051.07	K	Joback Method
tf	497.57	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.80	J/mol×K	847.17	Joback Method
cpg	1013.29	J/mol×K	881.15	Joback Method
cpg	1031.60	J/mol×K	915.14	Joback Method
cpg	1048.79	J/mol×K	949.12	Joback Method
cpg	1064.95	J/mol×K	983.10	Joback Method
cpg	1080.15	J/mol×K	1017.08	Joback Method
cpg	1094.46	J/mol×K	1051.07	Joback Method
dvisc	0.0040167	Pa×s	497.57	Joback Method

dvisc	0.0030980	Pa×s	555.84	Joback Method
dvisc	0.0025102	Pa×s	614.10	Joback Method
dvisc	0.0021094	Pa×s	672.37	Joback Method
dvisc	0.0018225	Pa×s	730.64	Joback Method
dvisc	0.0016090	Pa×s	788.90	Joback Method
dvisc	0.0014450	Pa×s	847.17	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=U391342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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