

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

Inchi: InChI=1S/C22H36O4/c1-3-5-6-15(4-2)14-25-20(23)7-8-21(24)26-22-18-10-16-9-17(12-18)
InchiKey: MVSDJCDMDZYYGI-UHFFFAOYSA-N
Formula: C22H36O4
SMILES: CCCCC(CC)COC(=O)CCC(=O)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-181.19	kJ/mol	Joback Method
hf	-820.73	kJ/mol	Joback Method
hfus	49.23	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.894		Crippen Method
mvol	303.140	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	2688.00		NIST Webbook
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tb	870.05	K	Joback Method
tc	1074.69	K	Joback Method
tf	508.84	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.46	J/molxK	870.05	Joback Method
cpg	1142.59	J/molxK	1040.58	Joback Method
cpg	1127.24	J/molxK	1006.48	Joback Method
cpg	1110.93	J/molxK	972.37	Joback Method
cpg	1093.58	J/molxK	938.26	Joback Method
cpg	1075.12	J/molxK	904.16	Joback Method
cpg	1157.06	J/molxK	1074.69	Joback Method
dvisc	0.0013209	Paxs	870.05	Joback Method

dvisc	0.0014795	Paxs	809.85	Joback Method
dvisc	0.0016875	Paxs	749.65	Joback Method
dvisc	0.0019696	Paxs	689.44	Joback Method
dvisc	0.0023677	Paxs	629.24	Joback Method
dvisc	0.0029595	Paxs	569.04	Joback Method
dvisc	0.0038996	Paxs	508.84	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=U391344&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

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