

Succinic acid, dodec-2-en-1-yl 3-methylbut-3-en-1-yl ester

Inchi:	InChI=1S/C21H36O4/c1-4-5-6-7-8-9-10-11-12-13-17-24-20(22)14-15-21(23)25-18-16-19
InchiKey:	NPIAVJISRRZGBH-OUKQBFOZSA-N
Formula:	C21H36O4
SMILES:	C=C(C)CCOC(=O)CCC(=O)OCC=CCCCCCCCC
Mol. weight [g/mol]:	352.51

Physical Properties

Property code	Value	Unit	Source
gf	-182.39	kJ/mol	Joback Method
hf	-733.51	kJ/mol	Joback Method
hfus	53.33	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.516		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1079.93	kPa	Joback Method
rinpol	2454.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	833.18	K	Joback Method
tc	1023.20	K	Joback Method
tf	449.95	K	Joback Method
vc	1.222	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.61	J/mol×K	833.18	Joback Method
cpg	994.23	J/mol×K	864.85	Joback Method
cpg	1010.84	J/mol×K	896.52	Joback Method
cpg	1026.46	J/mol×K	928.19	Joback Method
cpg	1041.13	J/mol×K	959.86	Joback Method
cpg	1054.89	J/mol×K	991.53	Joback Method
cpg	1067.76	J/mol×K	1023.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U391146&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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