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

Inchi: InChI=1S/C15H26O4/c1-5-7-13(6-2)19-15(17)9-8-14(16)18-11-10-12(3)4/h10,13H,5-9,11

InchiKey: QWNXFYFHFHZOBN-UHFFFAOYSA-N

Formula: C15H26O4

SMILES: CCCC(CC)OC(=O)CCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-323.19	kJ/mol	Joback Method
hf	-740.38	kJ/mol	Joback Method
hfus	35.55	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.398		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
tb	698.78	K	Joback Method
tc	883.94	K	Joback Method
tf	369.09	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.83	J/mol×K	698.78	Joback Method
cpg	670.84	J/mol×K	729.64	Joback Method
cpg	686.03	J/mol×K	760.50	Joback Method
cpg	700.43	J/mol×K	791.36	Joback Method
cpg	714.04	J/mol×K	822.22	Joback Method
cpg	726.87	J/mol×K	853.08	Joback Method
cpg	738.96	J/mol×K	883.94	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=U390548&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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