Succinic acid, 3-methylbut-2-en-1-yl 4-heptyl ester

Inchi: InChI=1S/C16H28O4/c1-5-7-14(8-6-2)20-16(18)10-9-15(17)19-12-11-13(3)4/h11,14H,5-1

InchiKey: YHIUJNHRXRNUMV-UHFFFAOYSA-N

Formula: C16H28O4

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

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-314.77	kJ/mol	Joback Method
hf	-761.02	kJ/mol	Joback Method
hfus	38.14	kJ/mol	Joback Method
hvap	69.17	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.788		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	721.66	K	Joback Method
tc	906.27	K	Joback Method
tf	380.36	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.57	J/mol×K	721.66	Joback Method
cpg	726.98	J/mol×K	752.43	Joback Method
cpg	742.54	J/mol×K	783.20	Joback Method
cpg	757.26	J/mol×K	813.96	Joback Method
cpg	771.17	J/mol×K	844.73	Joback Method
cpg	784.28	J/mol×K	875.50	Joback Method
cpg	796.60	J/mol×K	906.27	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=U390470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume