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

Inchi: InChI=1S/C16H28O4/c1-5-6-7-8-14(4)20-16(18)10-9-15(17)19-12-11-13(2)3/h14H,2,5-12

InchiKey: ZSHJRVQCYFPZCT-UHFFFAOYSA-N

Formula: C16H28O4

SMILES: C=C(C)CCOC(=O)CCC(=O)OC(C)CCCCC

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-307.15	kJ/mol	Joback Method
hf	-752.81	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	68.54	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.788		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	714.18	K	Joback Method
tc	895.85	K	Joback Method
tf	383.68	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.19	J/mol×K	714.18	Joback Method
cpg	725.58	J/mol×K	744.46	Joback Method
cpg	741.14	J/mol×K	774.74	Joback Method
cpg	755.86	J/mol×K	805.02	Joback Method
cpg	769.76	J/mol×K	835.30	Joback Method
cpg	782.86	J/mol×K	865.57	Joback Method
cpg	795.16	J/mol×K	895.85	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=U391135&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