Succinic acid, (adamant-1-yl)methyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C20H32O4/c1-13(2)14(3)24-19(22)5-4-18(21)23-12-20-9-15-6-16(10-20)8-17(7

InchiKey: HPDUAQGPKXTRIQ-UHFFFAOYSA-N

Formula: C20H32O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)OCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 336.47

Physical Properties

Property code	Value	Unit	Source
gf	-198.25	kJ/mol	Joback Method
hf	-749.15	kJ/mol	Joback Method
hfus	33.16	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.114		Crippen Method
mcvol	274.960	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	828.76	K	Joback Method
tc	1039.69	K	Joback Method
tf	499.44	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.99	J/mol×K	828.76	Joback Method
cpg	946.66	J/mol×K	863.92	Joback Method
cpg	966.70	J/mol×K	899.07	Joback Method
cpg	986.28	J/mol×K	934.23	Joback Method
cpg	1005.56	J/mol×K	969.38	Joback Method
cpg	1024.71	J/mol×K	1004.54	Joback Method
cpg	1043.89	J/mol×K	1039.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391354&Units=SI
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

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