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

Inchi: InChI=1S/C21H34O4/c1-14(2)15(3)25-20(23)5-4-19(22)24-7-6-21-11-16-8-17(12-21)10-1

InchiKey: PGOPWQYCCIRYDI-UHFFFAOYSA-N

Formula: C21H34O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-189.83	kJ/mol	Joback Method
hf	-769.79	kJ/mol	Joback Method
hfus	35.75	kJ/mol	Joback Method
hvap	78.33	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.504		Crippen Method
mcvol	289.050	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2592.00		NIST Webbook
rinpol	2592.00		NIST Webbook
tb	851.64	K	Joback Method
tc	1061.80	K	Joback Method
tf	510.71	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.42	J/mol×K	851.64	Joback Method
cpg	1008.55	J/mol×K	886.67	Joback Method
cpg	1029.10	J/mol×K	921.69	Joback Method
cpg	1049.25	J/mol×K	956.72	Joback Method
cpg	1069.16	J/mol×K	991.75	Joback Method
cpg	1089.00	J/mol×K	1026.78	Joback Method
cpg	1108.93	J/mol×K	1061.80	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=U391363&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