Succinic acid, 2-fluorophenyl adamant-2-yl ester

Inchi: InChI=1S/C20H23FO4/c21-16-3-1-2-4-17(16)24-18(22)5-6-19(23)25-20-14-8-12-7-13(10

InchiKey: ALHQRKCSXOEQPV-UHFFFAOYSA-N

Formula: C20H23FO4

SMILES: O=C(CCC(=O)OC1C2CC3CC(C2)CC1C3)Oc1ccccc1F

Mol. weight [g/mol]: 346.39

Physical Properties

Property code	Value	Unit	Source
gf	-287.62	kJ/mol	Joback Method
hf	-745.22	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	79.84	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.879		Crippen Method
mcvol	252.970	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	2699.00		NIST Webbook
tb	855.66	K	Joback Method
tc	1077.90	K	Joback Method
tf	540.83	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.31	J/mol×K	855.66	Joback Method
cpg	863.29	J/mol×K	892.70	Joback Method
cpg	879.06	J/mol×K	929.74	Joback Method
cpg	893.72	J/mol×K	966.78	Joback Method
cpg	907.36	J/mol×K	1003.82	Joback Method
cpg	920.09	J/mol×K	1040.86	Joback Method
cpg	932.00	J/mol×K	1077.90	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=U391343&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