

Succinic acid, hept-2-yl 4-acetylphenyl ester

Inchi: InChI=1S/C19H26O5/c1-4-5-6-7-14(2)23-18(21)12-13-19(22)24-17-10-8-16(9-11-17)15(3)
InchiKey: DLAJRXXVRC SIPB-UHFFFAOYSA-N
Formula: C19H26O5
SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-387.32	kJ/mol	Joback Method
hf	-817.89	kJ/mol	Joback Method
hfus	42.27	kJ/mol	Joback Method
hvap	85.50	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.087		Crippen Method
mvol	271.260	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	871.79	K	Joback Method
tc	1080.92	K	Joback Method
tf	522.08	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.98	J/molxK	871.79	Joback Method
cpg	850.22	J/molxK	906.65	Joback Method
cpg	863.28	J/molxK	941.50	Joback Method
cpg	875.17	J/molxK	976.36	Joback Method
cpg	885.92	J/molxK	1011.21	Joback Method
cpg	895.55	J/molxK	1046.07	Joback Method
cpg	904.08	J/molxK	1080.92	Joback Method
dvisc	0.0006006	Paxs	522.08	Joback Method
dvisc	0.0003307	Paxs	580.36	Joback Method

dvisc	0.0002030	Paxs	638.65	Joback Method
dvisc	0.0001352	Paxs	696.93	Joback Method
dvisc	0.0000959	Paxs	755.22	Joback Method
dvisc	0.0000715	Paxs	813.50	Joback Method
dvisc	0.0000554	Paxs	871.79	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=U389911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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