

Succinic acid, 2-ethylhexyl 4-acetylphenyl ester

Inchi:	InChI=1S/C20H28O5/c1-4-6-7-16(5-2)14-24-19(22)12-13-20(23)25-18-10-8-17(9-11-18)
InchiKey:	HVGDOPFJKOQUNL-UHFFFAOYSA-N
Formula:	C20H28O5
SMILES:	CCCCC(CC)COC(=O)CCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	348.43

Physical Properties

Property code	Value	Unit	Source
gf	-378.90	kJ/mol	Joback Method
hf	-838.53	kJ/mol	Joback Method
hfus	44.86	kJ/mol	Joback Method
hvap	87.72	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.334		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinsol	2671.00		NIST Webbook
tb	894.67	K	Joback Method
tc	1104.53	K	Joback Method
tf	533.35	K	Joback Method
vc	1.095	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.53	J/molxK	894.67	Joback Method
cpg	908.92	J/molxK	929.65	Joback Method
cpg	922.09	J/molxK	964.62	Joback Method
cpg	934.05	J/molxK	999.60	Joback Method
cpg	944.83	J/molxK	1034.58	Joback Method
cpg	954.45	J/molxK	1069.55	Joback Method
cpg	962.93	J/molxK	1104.53	Joback Method
dvisc	0.0005397	Paxs	533.35	Joback Method
dvisc	0.0002938	Paxs	593.57	Joback Method

dvisc	0.0001789	Paxs	653.79	Joback Method
dvisc	0.0001185	Paxs	714.01	Joback Method
dvisc	0.0000836	Paxs	774.23	Joback Method
dvisc	0.0000621	Paxs	834.45	Joback Method
dvisc	0.0000480	Paxs	894.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U389912&Units=SI

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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