

Succinic acid, 2-methylpent-3-yl 4-biphenyl ester

Inchi:	InChI=1S/C22H26O4/c1-4-20(16(2)3)26-22(24)15-14-21(23)25-19-12-10-18(11-13-19)17
InchiKey:	AQKPANRJECHOFH-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	CCC(OC(=O)CCC(=O)Oc1ccc(-c2ccccc2)cc1)C(C)C
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-123.17	kJ/mol	Joback Method
hf	-535.98	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	87.32	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.017		Crippen Method
mvol	288.200	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2815.00		NIST Webbook
rinpol	2815.00		NIST Webbook
tb	912.80	K	Joback Method
tc	1139.10	K	Joback Method
tf	517.38	K	Joback Method
vc	1.087	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.83	J/mol×K	912.80	Joback Method
cpg	913.38	J/mol×K	950.52	Joback Method
cpg	926.53	J/mol×K	988.23	Joback Method
cpg	938.32	J/mol×K	1025.95	Joback Method
cpg	948.81	J/mol×K	1063.67	Joback Method
cpg	958.04	J/mol×K	1101.39	Joback Method
cpg	966.05	J/mol×K	1139.10	Joback Method
dvisc	0.0005200	Paxs	517.38	Joback Method

dvisc	0.0002580	Paxs	583.28	Joback Method
dvisc	0.0001476	Paxs	649.19	Joback Method
dvisc	0.0000936	Paxs	715.09	Joback Method
dvisc	0.0000641	Paxs	780.99	Joback Method
dvisc	0.0000465	Paxs	846.90	Joback Method
dvisc	0.0000354	Paxs	912.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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