

Succinic acid, 2-methylpent-3-yl 2-methoxyphenyl ester

Inchi: InChI=1S/C17H24O5/c1-5-13(12(2)3)21-16(18)10-11-17(19)22-15-9-7-6-8-14(15)20-4/h6
InchiKey: NKLULSNWHHFGCW-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: CCC(OC(=O)CCC(=O)Oc1ccccc1OC)C(C)C
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-382.68	kJ/mol	Joback Method
hf	-801.53	kJ/mol	Joback Method
hfus	33.15	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.359		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	794.14	K	Joback Method
tc	999.34	K	Joback Method
tf	456.84	K	Joback Method
vc	0.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.78	J/molxK	794.14	Joback Method
cpg	749.16	J/molxK	828.34	Joback Method
cpg	763.42	J/molxK	862.54	Joback Method
cpg	776.55	J/molxK	896.74	Joback Method
cpg	788.57	J/molxK	930.94	Joback Method
cpg	799.47	J/molxK	965.14	Joback Method
cpg	809.25	J/molxK	999.34	Joback Method
dvisc	0.0007302	Paxs	456.84	Joback Method

dvisc	0.0003706	Paxs	513.06	Joback Method
dvisc	0.0002151	Paxs	569.27	Joback Method
dvisc	0.0001376	Paxs	625.49	Joback Method
dvisc	0.0000948	Paxs	681.71	Joback Method
dvisc	0.0000691	Paxs	737.92	Joback Method
dvisc	0.0000527	Paxs	794.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389705&Units=SI
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

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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