

Succinic acid, cyclohexylmethyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H28O5/c25-23(27-17-19-8-3-1-4-9-19)14-15-24(26)28-18-20-10-7-13-22(1)
InchiKey: YRLJIYCLNWDJBM-UHFFFAOYSA-N
Formula: C24H28O5
SMILES: O=C(CCC(=O)OCC1CCCCC1)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 396.48

Physical Properties

Property code	Value	Unit	Source
gf	-182.00	kJ/mol	Joback Method
hf	-644.60	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	95.38	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.426		Crippen Method
mcvol	311.390	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	1001.41	K	Joback Method
tc	1241.70	K	Joback Method
tf	599.53	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.53	J/mol×K	1001.41	Joback Method
cpg	1083.13	J/mol×K	1201.65	Joback Method
cpg	1077.39	J/mol×K	1161.60	Joback Method
cpg	1069.91	J/mol×K	1121.55	Joback Method
cpg	1060.64	J/mol×K	1081.51	Joback Method
cpg	1049.53	J/mol×K	1041.46	Joback Method
cpg	1087.18	J/mol×K	1241.70	Joback Method
dvisc	0.0000242	Pa×s	1001.41	Joback Method

dvisc	0.0000312	Pa×s	934.43	Joback Method
dvisc	0.0000419	Pa×s	867.45	Joback Method
dvisc	0.0000591	Pa×s	800.47	Joback Method
dvisc	0.0000888	Pa×s	733.49	Joback Method
dvisc	0.0001448	Pa×s	666.51	Joback Method
dvisc	0.0002634	Pa×s	599.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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