

Glutaric acid, hept-2-yl diphenylmethyl ester

Inchi: InChI=1S/C25H32O4/c1-3-4-7-13-20(2)28-23(26)18-12-19-24(27)29-25(21-14-8-5-9-15-20)
InchiKey: QIMGWYNZEPQLDB-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-88.28	kJ/mol	Joback Method
hf	-586.43	kJ/mol	Joback Method
hfus	47.12	kJ/mol	Joback Method
hvap	93.33	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.002		Crippen Method
mvol	330.470	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rmpol	2808.00		NIST Webbook
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tb	976.46	K	Joback Method
tc	1202.47	K	Joback Method
tf	538.67	K	Joback Method
vc	1.256	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.81	J/molxK	976.46	Joback Method
cpg	1138.45	J/molxK	1164.80	Joback Method
cpg	1129.15	J/molxK	1127.13	Joback Method
cpg	1118.61	J/molxK	1089.46	Joback Method
cpg	1106.75	J/molxK	1051.80	Joback Method
cpg	1093.50	J/molxK	1014.13	Joback Method
cpg	1146.56	J/molxK	1202.47	Joback Method
dvisc	0.0000222	Paxs	976.46	Joback Method

dvisc	0.0000298	Paxs	903.50	Joback Method
dvisc	0.0000420	Paxs	830.53	Joback Method
dvisc	0.0000634	Paxs	757.57	Joback Method
dvisc	0.0001043	Paxs	684.60	Joback Method
dvisc	0.0001934	Paxs	611.64	Joback Method
dvisc	0.0004239	Paxs	538.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393344&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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