

Glutaric acid, 2-methylpent-3-yl diphenylmethyl ester

Inchi:	InChI=1S/C24H30O4/c1-4-21(18(2)3)27-22(25)16-11-17-23(26)28-24(19-12-7-5-8-13-19
InchiKey:	CFFHYFQSHRAARU-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	CCC(OC(=O)CCCC(=O)OC(c1ccccc1)c1ccccc1)C(C)C
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-99.14	kJ/mol	Joback Method
hf	-571.07	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	90.72	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.467		Crippen Method
mvol	316.380	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2687.00		NIST Webbook
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tb	953.14	K	Joback Method
tc	1180.00	K	Joback Method
tf	512.40	K	Joback Method
vc	1.194	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.06	J/molxK	953.14	Joback Method
cpg	1033.80	J/molxK	990.95	Joback Method
cpg	1047.09	J/molxK	1028.76	Joback Method
cpg	1058.98	J/molxK	1066.57	Joback Method
cpg	1069.53	J/molxK	1104.38	Joback Method
cpg	1078.82	J/molxK	1142.19	Joback Method
cpg	1086.89	J/molxK	1180.00	Joback Method
dvisc	0.0005477	Paxs	512.40	Joback Method

dvisc	0.0002333	Paxs	585.86	Joback Method
dvisc	0.0001202	Paxs	659.31	Joback Method
dvisc	0.0000707	Paxs	732.77	Joback Method
dvisc	0.0000459	Paxs	806.23	Joback Method
dvisc	0.0000320	Paxs	879.68	Joback Method
dvisc	0.0000235	Paxs	953.14	Joback Method

Sources

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=U393341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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