

Glutaric acid, 8-chlorooctyl 4-biphenyl ester

Inchi:	InChI=1S/C25H31ClO4/c26-19-8-3-1-2-4-9-20-29-24(27)13-10-14-25(28)30-23-17-15-22
InchiKey:	TZGPSJWHAVGYCI-UHFFFAOYSA-N
Formula:	C25H31ClO4
SMILES:	O=C(CCCC(=O)Oc1ccc(-c2ccccc2)cc1)OCCCCCCCCI
Mol. weight [g/mol]:	430.96

Physical Properties

Property code	Value	Unit	Source
gf	-104.96	kJ/mol	Joback Method
hf	-603.08	kJ/mol	Joback Method
hfus	57.97	kJ/mol	Joback Method
hvap	99.15	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.552		Crippen Method
mvol	342.710	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
rinpol	3496.00		NIST Webbook
rinpol	3496.00		NIST Webbook
tb	1019.75	K	Joback Method
tc	1250.65	K	Joback Method
tf	611.11	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.67	J/molxK	1019.75	Joback Method
cpg	1112.87	J/molxK	1058.23	Joback Method
cpg	1124.65	J/molxK	1096.72	Joback Method
cpg	1135.09	J/molxK	1135.20	Joback Method
cpg	1144.25	J/molxK	1173.68	Joback Method
cpg	1152.19	J/molxK	1212.16	Joback Method
cpg	1158.98	J/molxK	1250.65	Joback Method
dvisc	0.0002431	Paxs	611.11	Joback Method

dvisc	0.0001350	Paxs	679.22	Joback Method
dvisc	0.0000834	Paxs	747.32	Joback Method
dvisc	0.0000558	Paxs	815.43	Joback Method
dvisc	0.0000398	Paxs	883.54	Joback Method
dvisc	0.0000297	Paxs	951.64	Joback Method
dvisc	0.0000231	Paxs	1019.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390131&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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