

Glutaric acid, 2-isopropoxyphenyl tetradecyl ester

Inchi:	InChI=1S/C28H46O5/c1-4-5-6-7-8-9-10-11-12-13-14-17-23-31-27(29)21-18-22-28(30)33
InchiKey:	LAJXSYBMXDGQAX-UHFFFAOYSA-N
Formula:	C28H46O5
SMILES:	CCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]:	462.66

Physical Properties

Property code	Value	Unit	Source
gf	-287.62	kJ/mol	Joback Method
hf	-1023.29	kJ/mol	Joback Method
hfus	65.17	kJ/mol	Joback Method
hvap	101.19	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.794		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinpol	3312.00		NIST Webbook
rinpol	3312.00		NIST Webbook
tb	1046.26	K	Joback Method
tc	1287.87	K	Joback Method
tf	595.81	K	Joback Method
vc	1.556	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.63	J/molxK	1046.26	Joback Method
cpg	1415.70	J/molxK	1086.53	Joback Method
cpg	1430.69	J/molxK	1126.80	Joback Method
cpg	1443.65	J/molxK	1167.06	Joback Method
cpg	1454.64	J/molxK	1207.33	Joback Method
cpg	1463.72	J/molxK	1247.60	Joback Method
cpg	1470.93	J/molxK	1287.87	Joback Method
dvisc	0.0001768	Paxs	595.81	Joback Method

dvisc	0.0000862	Paxs	670.88	Joback Method
dvisc	0.0000486	Paxs	745.96	Joback Method
dvisc	0.0000304	Paxs	821.03	Joback Method
dvisc	0.0000206	Paxs	896.11	Joback Method
dvisc	0.0000148	Paxs	971.18	Joback Method
dvisc	0.0000111	Paxs	1046.26	Joback Method

Sources

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=U358580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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