

Glutaric acid, 2,3-dimethylphenyl pentadecyl ester

Inchi:	InChI=1S/C28H46O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-23-31-27(29)21-18-22-28(30)
InchiKey:	QEEZOURDZKKGMX-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	446.66

Physical Properties

Property code	Value	Unit	Source
gf	-189.81	kJ/mol	Joback Method
hf	-897.26	kJ/mol	Joback Method
hfus	67.11	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.014		Crippen Method
mvol	396.500	ml/mol	McGowan Method
pc	810.30	kPa	Joback Method
rinpol	3393.00		NIST Webbook
rinpol	3393.00		NIST Webbook
tb	1029.26	K	Joback Method
tc	1265.35	K	Joback Method
tf	601.10	K	Joback Method
vc	1.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1368.97	J/molxK	1029.26	Joback Method
cpg	1387.04	J/molxK	1068.61	Joback Method
cpg	1403.28	J/molxK	1107.96	Joback Method
cpg	1417.75	J/molxK	1147.31	Joback Method
cpg	1430.51	J/molxK	1186.65	Joback Method
cpg	1441.62	J/molxK	1226.00	Joback Method
cpg	1451.15	J/molxK	1265.35	Joback Method
dvisc	0.0002098	Paxs	601.10	Joback Method

dvisc	0.0001109	Paxs	672.46	Joback Method
dvisc	0.0000662	Paxs	743.82	Joback Method
dvisc	0.0000433	Paxs	815.18	Joback Method
dvisc	0.0000303	Paxs	886.54	Joback Method
dvisc	0.0000223	Paxs	957.90	Joback Method
dvisc	0.0000172	Paxs	1029.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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