

Glutaric acid, naphth-2-ylmethyl 2-propylphenyl ester

Inchi:	InChI=1S/C25H26O4/c1-2-8-21-10-5-6-12-23(21)29-25(27)14-7-13-24(26)28-18-19-15-1
InchiKey:	FYXFHVIWFIQVJA-UHFFFAOYSA-N
Formula:	C25H26O4
SMILES:	CCCc1ccccc1OC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	390.47

Physical Properties

Property code	Value	Unit	Source
gf	3.99	kJ/mol	Joback Method
hf	-407.74	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	97.07	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	5.611		Crippen Method
mcvol	311.010	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	3264.00		NIST Webbook
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tb	1006.28	K	Joback Method
tc	1242.63	K	Joback Method
tf	626.41	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.44	J/molxK	1006.28	Joback Method
cpg	1047.09	J/molxK	1203.24	Joback Method
cpg	1038.20	J/molxK	1163.84	Joback Method
cpg	1028.38	J/molxK	1124.45	Joback Method
cpg	1017.54	J/molxK	1085.06	Joback Method
cpg	1005.59	J/molxK	1045.67	Joback Method
cpg	1055.13	J/molxK	1242.63	Joback Method
dvisc	0.0000593	Paxs	1006.28	Joback Method

dvisc	0.0000728	Paxs	942.97	Joback Method
dvisc	0.0000920	Paxs	879.66	Joback Method
dvisc	0.0001205	Paxs	816.35	Joback Method
dvisc	0.0001653	Paxs	753.03	Joback Method
dvisc	0.0002403	Paxs	689.72	Joback Method
dvisc	0.0003766	Paxs	626.41	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=U392151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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