

Glutaric acid, hex-4-yn-3-yl 2-propylphenyl ester

Inchi:	InChI=1S/C20H26O4/c1-4-10-16-12-7-8-13-18(16)24-20(22)15-9-14-19(21)23-17(6-3)11
InchiKey:	GZBXYSMYWRCXCN-UHFFFAOYSA-N
Formula:	C20H26O4
SMILES:	CC#CC(CC)OC(=O)CCCC(=O)Oc1ccccc1CCC
Mol. weight [g/mol]:	330.42

Physical Properties

Property code	Value	Unit	Source
gf	-47.18	kJ/mol	Joback Method
hf	-453.65	kJ/mol	Joback Method
hfus	46.38	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.060		Crippen Method
mcvol	275.180	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpola	2314.00		NIST Webbook
rinpola	2314.00		NIST Webbook
tb	849.80	K	Joback Method
tc	1064.28	K	Joback Method
tf	589.52	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.60	J/mol×K	849.80	Joback Method
cpg	842.18	J/mol×K	885.55	Joback Method
cpg	856.55	J/mol×K	921.29	Joback Method
cpg	869.73	J/mol×K	957.04	Joback Method
cpg	881.75	J/mol×K	992.79	Joback Method
cpg	892.63	J/mol×K	1028.53	Joback Method
cpg	902.38	J/mol×K	1064.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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