

Glutaric acid, hept-2-yl 4-chloro-2-methoxyphenyl ester

Inchi:	InChI=1S/C19H27ClO5/c1-4-5-6-8-14(2)24-18(21)9-7-10-19(22)25-16-12-11-15(20)13-17
InchiKey:	IXSYWCHIWWGRJX-UHFFFAOYSA-N
Formula:	C19H27ClO5
SMILES:	CCCCC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	370.87

Physical Properties

Property code	Value	Unit	Source
gf	-384.96	kJ/mol	Joback Method
hf	-864.74	kJ/mol	Joback Method
hfus	45.66	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.936		Crippen Method
mvol	287.800	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	2536.00		NIST Webbook
rinpol	2536.00		NIST Webbook
tb	882.75	K	Joback Method
tc	1090.87	K	Joback Method
tf	536.82	K	Joback Method
vc	1.101	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.18	J/molxK	882.75	Joback Method
cpg	932.97	J/molxK	1056.18	Joback Method
cpg	923.67	J/molxK	1021.49	Joback Method
cpg	913.15	J/molxK	986.81	Joback Method
cpg	901.39	J/molxK	952.12	Joback Method
cpg	888.41	J/molxK	917.44	Joback Method
cpg	941.05	J/molxK	1090.87	Joback Method
dvisc	0.0000379	Paxs	882.75	Joback Method

dvisc	0.0000484	Paxs	825.10	Joback Method
dvisc	0.0000642	Paxs	767.44	Joback Method
dvisc	0.0000891	Paxs	709.78	Joback Method
dvisc	0.0001310	Paxs	652.13	Joback Method
dvisc	0.0002077	Paxs	594.47	Joback Method
dvisc	0.0003635	Paxs	536.82	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=U393908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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