

Glutaric acid, butyl 2,4-dichloronaphthyl ester

Inchi: InChI=1S/C19H20Cl2O4/c1-2-3-11-24-17(22)9-6-10-18(23)25-19-14-8-5-4-7-13(14)15(20)
InchiKey: LWBISMRTYZLPU-UHFFFAOYSA-N
Formula: C19H20Cl2O4
SMILES: CCCCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]: 383.27

Physical Properties

Property code	Value	Unit	Source
gf	-192.43	kJ/mol	Joback Method
hf	-563.38	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.566		Crippen Method
mcvol	274.710	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpola	2895.00		NIST Webbook
rinpola	2895.00		NIST Webbook
tb	922.16	K	Joback Method
tc	1146.56	K	Joback Method
tf	604.73	K	Joback Method
vc	1.060	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.19	J/molxK	922.16	Joback Method
cpg	801.04	J/molxK	959.56	Joback Method
cpg	811.87	J/molxK	996.96	Joback Method
cpg	821.73	J/molxK	1034.36	Joback Method
cpg	830.65	J/molxK	1071.76	Joback Method
cpg	838.69	J/molxK	1109.16	Joback Method
cpg	845.89	J/molxK	1146.56	Joback Method
dvisc	0.0004756	Paxs	604.73	Joback Method

dvisc	0.0003294	Paxs	657.63	Joback Method
dvisc	0.0002410	Paxs	710.54	Joback Method
dvisc	0.0001841	Paxs	763.45	Joback Method
dvisc	0.0001456	Paxs	816.35	Joback Method
dvisc	0.0001185	Paxs	869.26	Joback Method
dvisc	0.0000988	Paxs	922.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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