

Fumaric acid, naphth-1-yl 3-chlorophenyl ester

Inchi: InChI=1S/C20H13ClO4/c21-15-7-4-8-16(13-15)24-19(22)11-12-20(23)25-18-10-3-6-14-5
InchiKey: NEPIPLKTFAXJJO-VAWYXSNFSA-N
Formula: C20H13ClO4
SMILES: O=C(C=CC(=O)Oc1cccc2ccccc12)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 352.77

Physical Properties

Property code	Value	Unit	Source
gf	30.18	kJ/mol	Joback Method
hf	-203.06	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	90.28	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.560		Crippen Method
mcvol	248.500	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	2916.00		NIST Webbook
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tb	933.47	K	Joback Method
tc	1187.29	K	Joback Method
tf	594.90	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.23	J/molxK	933.47	Joback Method
cpg	704.16	J/molxK	975.77	Joback Method
cpg	714.09	J/molxK	1018.08	Joback Method
cpg	723.14	J/molxK	1060.38	Joback Method
cpg	731.40	J/molxK	1102.69	Joback Method
cpg	739.00	J/molxK	1144.99	Joback Method
cpg	746.04	J/molxK	1187.29	Joback Method
dvisc	0.0004738	Paxs	594.90	Joback Method

dvisc	0.0003177	Paxs	651.33	Joback Method
dvisc	0.0002270	Paxs	707.76	Joback Method
dvisc	0.0001705	Paxs	764.19	Joback Method
dvisc	0.0001332	Paxs	820.61	Joback Method
dvisc	0.0001074	Paxs	877.04	Joback Method
dvisc	0.0000889	Paxs	933.47	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=U405814&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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